

Comparison of the photoionisation modelling results for planetary nebulae with the observed data

*M. Kasheba**, *B. Ya. Melekh†*

Department of Astrophysics, Ivan Franko National University of Lviv, 8 Kyryla & Mephodiya str., Lviv, Ukraine

The grid of new photoionisation models for planetary nebulae (PNe) along the evolutionary tracks of their nuclei was calculated, taking into account the dust presence with abundances that correspond to the averaged ones for Milky Way and Large Magellanic Cloud. The calculations were performed by the last version of G. Ferland's code `Cloudy v17.01` using the semi-empirical law derived by Golovaty-Mal'kov to describe the radial density distribution of matter in the nebular envelope of PN. Resulting modelling spectra were compared with the corresponding observed emission line spectra of PNe in optical range, obtained previously by other authors. Also the database of observations by the Infrared Space Observatory and Spitzer have been used to compare the results of synthetic photometry with the observed photometric data. It was shown that the intensities of strong emission lines in optical range as well as the observed color-color diagrams obtained using total fluxes in the $3.6\ \mu\text{m}$, $4.5\ \mu\text{m}$, $8.0\ \mu\text{m}$ and $24.0\ \mu\text{m}$ bands are reproduced very well by our models, while the results of synthetic IR-photometry based on total fluxes in the band $5.8\ \mu\text{m}$ show discrepancies with corresponding observed data.

Key words: ISM: abundances, lines and bands; infrared: ISM

INTRODUCTION

Precise determination of the chemical abundances in planetary nebulae (PNe) is very important for study of chemical evolution of the Universe. Due to their relatively simple structure, their abundance can be determined with good precision. All methods to determine the chemical abundances are based on the diagnostic of PNe spectra [78]. But the emission lines of some ions are absent in PNe spectra. To solve this problem the photoionisation modelling (PhM) of their envelopes is usually used (see for an example [54, 55, 74, 79, 104]). In such modelling the radiative fluxes in most of the emission lines of all ions as well as all corresponding ionic abundances within the PNe envelope can be calculated. These data can be used to derive the expressions for the so-called ionisation-correction factors (ICFs) which allow to determine the full abundance of chemical elements within the PN envelope on base of the ionic one calculated via the diagnostic methods (see [79]). In our opinion the ICFs determination using PhM can be correct only under the condition that the modelling spectra reproduce the observed ones for corresponding nebular objects (in our case – PNe).

Also it is important to take into account the dust grains presence within the PN envelope. When the dust grains are cooling, they produce the grain ther-

mal emission (see e.g. [71, 80]) with the maximum in IR wavelength range. Measured continuum due to the dust emission gives the additional information on PNe.

In present work we calculate the advanced photoionisation models grid and compare its results with the observed data in optical and IR wavelength range.

In the next section the grid of photoionisation models is described. After that we compare the synthetic spectra from our PhM grid with the observed ones in optical and IR wavelength ranges and then make the conclusions.

DESCRIPTION OF PHOTOIONISATION MODELS GRID

We calculated the photoionisation models grid using the code `Cloudy 17.01` which includes the newest atomic data, bug fixes and improved computations [39]. As in [78] we calculated this grid along the evolutionary tracks of PNe nuclei for two various chemical abundance sets (gas and dust grains), averaged over the ones obtained during the previous investigations of PNe in Milky Way (MW) and Large Magellanic Cloud (LMC) correspondingly (see details in [78]). The density distribution in mod-

*liceistdominator@gmail.com

†bohdan.melekh@lnu.edu.ua

els was defined by Golovatyy & Mal'kov (GM) semi-empirical law [44]. Most details of the grid calculation can be found in [78], where the older version (08.00) of *CLOUDY* was used. Here we describe only some principal points.

All photoionisation models in the grid were calculated under the assumption of spherical symmetry. The Hydrogen density distribution within the PN envelope was described using GM semi-empirical law [44]:

$$n_H(r) = \frac{x^2(1 + 3e^{-1.2x})}{(x^2 - 1)^2 + 0.36r_c^{-0.43}x^2} \frac{A_{dens}}{r_c^2},$$

where $x = r/r_c$, r_c is the characteristic radius of PN, close to the position of maximal density; A_{dens} is the density parameter depending on the wind parameters during the PN formation (proportional to the mass loss rate and inversely proportional to the velocity of wind). Golovatyy & Mal'kov obtained this expression fitting the density distributions derived from the isophote maps of several real PNe with various sizes (ages) assuming the spherical symmetry. Photoionisation models grid was calculated for the following values of A_{dens} : [1.0; 8.0] with the step 0.25.

In [44] the most compact (youngest) nebula has the maximal density value of $100\,000\text{ cm}^{-3}$. Therefore we assumed this density for zero age ($t = 0$) at $r = r_c$. Characteristic radius r_c values were calculated as the function of time as $r_c = v_{exp} \cdot t$, where the velocity of expansion v_{exp} depends on the temperature of photosphere of PN nucleus: $v_{exp} = 10\text{ km/s}$ for $T_{eff} \leq 2 \cdot 10^4\text{ K}$ and $v_{exp} = 20\text{ km/s}$ for $T_{eff} > 2 \cdot 10^4\text{ K}$. Inner radius r_i is calculated using the approximation expression derived by fitting of the results obtained in [44]:

$$\frac{r_i}{r_c} = 0.440935 - 4.89604r_c + 27.9594r_c^2 - 44.0096r_c^3.$$

Mass of the PN nucleus was calculated by Vassiliadis & Woodes relation [107]:

$$\frac{M_n}{M_\odot} = 0.473 + 0.084 \frac{M_0}{M_\odot} - 0.058 \log \frac{Z}{Z_\odot}$$

Outer radius r_o of the PN envelope was calculated using the following condition:

$$\int_{r_i}^{r_o} n_H(r) \cdot 4\pi r^2 m_H dr \equiv M_{env} = M_0 - M_n,$$

where M_{env} is the PN envelope mass determined as difference between the mass of progenitor star (M_0) and the mass of nucleus of PNe (M_n).

Grid was calculated for two different types of the dust particles (carbonates and silicates) with abundances corresponding to the averaged ones for Milky Way and LMC correspondingly (see [71, 78]).

To define the *Lyc*-spectrum from a central star in our models we selected progenitor stars with the masses of 0.95, 1.00 and 1.50 Solar masses [78]. A part of the progenitor star mass will be blown into the PN envelope and the rest will stay in the PN nucleus that becomes a white dwarf (source of the ionising radiation).

Models were calculated along the evolutionary tracks of central stars (nuclei of PNe). Their evolution is described by the evolutionary tracks from [107]. You can find the evolutionary tracks used in our models in paper [78].

COMPARISON OF MODELS WITH OBSERVATIONS

To be sure that our models describe the real PNe, we checked them on reproducing of the corresponding observed data. For this purpose we compare: (i) the resulting modelling intensities of the so-called strong emission lines (observed in each of PNe) in optical wavelength range with the observed ones; (ii) the modelling color-color diagrams obtained as result of the synthetic photometry of the modelling IR-spectra with the results of photometric observations by the Infrared Space Observatory (ISO) and Spitzer space telescopes (see details below).

We used for comparison with the observed data on PNe in optical wavelength range intensities of the following strong emission lines:

$$R_3 = [\text{O III}] 5007 / H_\beta;$$

$$R_2 = ([\text{O II}] 3727 + [\text{O III}] 3729) / H_\beta;$$

$$N_2 = [\text{N II}] 6548 / H_\beta;$$

$$S_2 = ([\text{S II}] 6717 + [\text{S II}] 6731) / H_\beta.$$

In Fig.4 we compare the modelling intensities of strong emission lines with the observed ones from the set by Mal'kov from [1–38, 40–43, 45, 46, 48–53, 58–70, 72, 73, 75–77, 81–102, 105, 106, 108].

Big solid circles represent the observed data, while all other symbols correspond to our models. 'H' and 'He' denoted in brackets mean different types of nuclear burning within the outer shell of PN nucleus. In these diagrams the modeling results (starting from the models at zero age until 50 000 years) corresponding to all mentioned above values of the density parameter A_{dens} in the GM density distribution and both types of the grain particles are shown. It can be seen that the strong emission lines from our models coincide with the corresponding observed

¹http://general-tools.cosmos.esa.int/iso/manuals/HANDBOOK/gen_hb/gen_hb.pdf

data. It means that the models of our grid reproduce very well the optical emission line spectra.

Our modelling results in IR were compared with the following observed data: the synthetic photometry of the ISO spectra¹ of PNe in Milky Way [71, 103] and the observed photometric data on PNe in Large Magellanic Cloud obtained by the Spitzer Space Telescope during the Surveying the Agents of a Galaxy Evolution (SAGE) program [56]. We used bands of the Spitzer instruments IRAC (Infrared Array Camera) and MIPS (Multiband Imaging Photometer). IRAC provides 4 bands for the photometric observations (3.6 μm , 4.5 μm , 5.8 μm , 8.0 μm), while from MIPS we used only one band – 24.0 μm .

Total fluxes (or magnitudes) in different photometric bands were calculated as in [57] taking into account the sensitivity curves for corresponding devices described in [56] and MIPS Instrument Handbook². For example:

$$\begin{aligned} [8.0] - [24.0] &\equiv m_{8.0\mu\text{m}} - m_{24.0\mu\text{m}} = \\ &= 2.5 \log \left(\frac{F_{24.0\mu\text{m}}}{F_{8.0\mu\text{m}}} * \frac{F_{0,8.0\mu\text{m}}}{F_{0,24.0\mu\text{m}}} \right), \end{aligned}$$

where $F_{0,\lambda}$ denotes the flux for zero-point magnitude in λ band [47]. In our diagrams we labeled the wavelengths in brackets as the value of magnitude in the corresponding photometric band.

Color-color diagrams in Fig. 2 represent the models for progenitor star with the mass of $1.0 M_{\odot}$. We do not show the models for other values of the progenitor star masses, because they show similar behaviour in these color-color diagrams. In these figures the models of PNe in LMC and MW are shown for the values of density parameter $A = 1.0$ and $A = 8.0$ (marginal values) consisting of two dust grain types: silicates (sil) and carbonates (ac1). The models with intermediate values of the parameter A lay between the tracks of these parameters, therefore we do not show them. Models for LMC were calculated for progenitor stars with the masses of $0.95 M_{\odot}$, $1.0 M_{\odot}$ and $1.5 M_{\odot}$. As in [71, 78] for the models of PNe in LMC we applied the dust grains factors of 0.74 for carbonates and 0.25 for silicates for the corresponding abundances adopted by default in the code *CLOUDY* [39]. In the models of PNe in MW calculated for progenitor stars with the masses of $1.0 M_{\odot}$ and $1.5 M_{\odot}$ the dust grains factor values of 1.07 and 0.52 for carbonates and silicates respectively [71, 78] were adopted.

It must be noted that the behaviour of diagrams color-color differs for various types of dust: while the models with carbonates dust grains fit better the observed diagram [4.5]–[8.0] versus [3.6]–[4.5], the ones with silicates fit reasonably well the observed dia-

gram [8.0]–[24.0] versus [3.6]–[8.0]. Also in the diagram [4.5]–[8.0] versus [3.6]–[4.5] some observed data for MW not covered by our models can be seen. Figures show the good overlap with the observed data of the modelling color-color diagrams, obtained using total fluxes in the 3.6 μm , 4.5 μm , 8.0 μm and 24.0 μm bands.

Also, in Fig. 2 the main problem of our models can be seen: the modelling total fluxes in the 5.8 μm band are underestimated in comparison with the observed ones. Trying to solve this problem we changed our models. The initial (for zero age) value of density $n_{\text{H}}(r_c)$ was varied within the range from $50\,000\text{ cm}^{-3}$ to $500\,000\text{ cm}^{-3}$. The resulting color-color diagrams can be found on the web page³. From the analysis of results it was concluded that such variations change the track of our models in color-color diagram only slightly. The character of the r_c and, correspondingly, r_i evolution was changed. For this purpose the radii shift factor was introduced. The adopted values of this parameter are: 0.8, 1.0, 1.5. The resulting color-color diagrams can be found on the web page⁴. The main conclusion is that the changes in r_c have larger impact on the modelling results than the ones in $n_{\text{H}}(r_c)$, but they are still not enough to solve the problem with flux at 5.8 μm .

We were testing the dust factors values of 0.01, 0.05, 0.1, 0.5, 1.0 and 2.0 to deviate the abundances of both types of dust particles from the adopted in code *CLOUDY* by default [39]. Dust abundance changes have much more significant impact on the tracks of our PhM results in color-color diagrams than the previous ones. In Fig. 3 it is shown how the dust abundance variation changes the position of evolutionary sequence of the modelling results in color-color diagrams for the models of PNe in MW with the carbonates dust grains at $A = 8.0$ and the PN progenitor mass of $1.0 M_{\odot}$. The models for silicate dust at other values of the parameter A and PN progenitor mass as well as for PNe in LMC do not change the main conclusion, therefore we do not show them in these figures. It can be seen that the change of this parameter value allows to cover by models most of the regions of the observed data in these diagrams, except for the ones where flux at 5.8 μm is involved as well as the diagram [4.5]–[8.0] versus [3.6]–[4.5] where some part of the observed data region for MW is not covered by our models. Thus, unfortunately, such models also do not solve the problem with underestimation of the total flux at 5.8 μm by our PhM.

CONCLUSIONS

The new photoionisation models grid for PNe in MW and LMC along the evolutionary tracks of their

²<https://irsa.ipac.caltech.edu/data/SPITZER/docs/mips/mipsinstrumenthandbook/>

³http://physics.lnu.edu.ua/wp-content/uploads/Change_nrc.pdf

⁴http://physics.lnu.edu.ua/wp-content/uploads/Change_rc.pdf

nuclei with the radial density distribution defined by Golovaty & Mal'kov (GM) semi-empirical law [44] was calculated using the code `Cloudy` 17.01 (newest version of code at present). The resulting modelling emission line spectra in optical wavelength region as well as the results of synthetic photometry of models in IR were compared with the corresponding observed data. From this comparison we obtained the following conclusions:

1. The results of our PhM of PNe envelopes show the good overlap with the data of spectroscopic observations in optical wavelength region;
2. We obtained the good coverage of the observed IR color-color diagrams by the modelling ones formed using total fluxes in the $3.6\ \mu\text{m}$, $4.5\ \mu\text{m}$, $8.0\ \mu\text{m}$ and $24.0\ \mu\text{m}$ bands;
3. In the diagram $[4.5]-[8.0]$ versus $[3.6]-[4.5]$ some observed data for PNe in MW are not covered by our models. Thus, the task of search of the additional models of PNe in MW, which would cover this observed data region, arises;
4. Color-color diagrams obtained using the total flux in the $5.8\ \mu\text{m}$ band do not reproduce the corresponding observed ones: the values of total modelling flux of radiation in this band are lower than the ones obtained by the IR space telescopes Spitzer [56] and ISO [71, 103]. The variations of dust abundance as well as the parameters which define the evolution of density distribution do not solve this problem. Is it a problem of models or observations? Why do the modelling fluxes allow to reproduce the observed color-color diagram in all the bands, except for the $5.8\ \mu\text{m}$ one?

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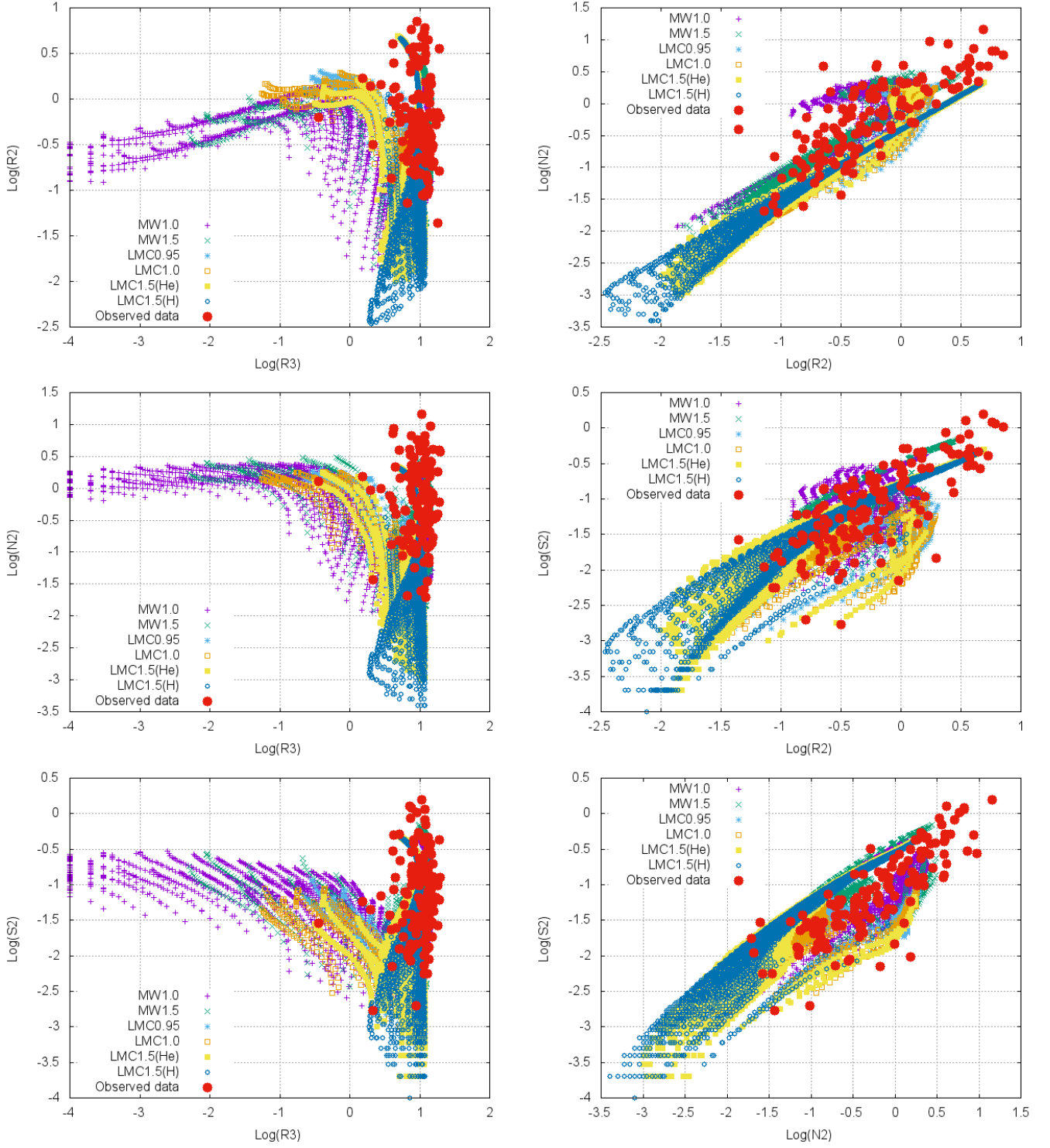


Fig. 1: Comparison of the modelling intensities of the optical strong emission lines, obtained from PhM of PNe in MW and LMC calculated for the progenitor stars of $0.95M_{\odot}$, $1.0M_{\odot}$ and $1.5M_{\odot}$, with the corresponding observed data (see description in the text).

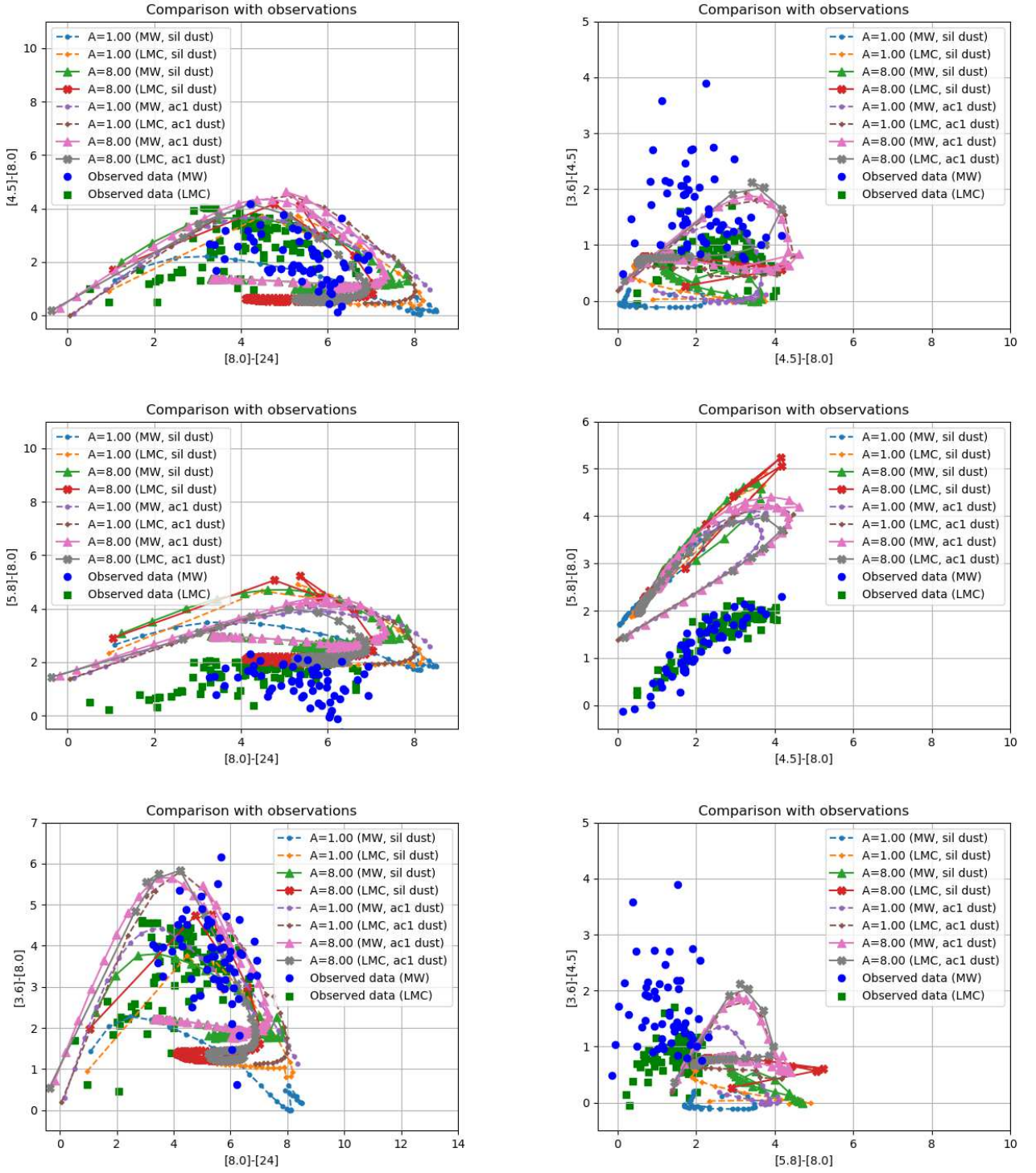


Fig. 2: Comparison of the modelling color-color diagrams, obtained using the synthetic photometry (see description in the text) of IR spectra from PhM of PNe in MW and LMC with the mass of progenitor star of $1.0M_{\odot}$, with the observed ones.

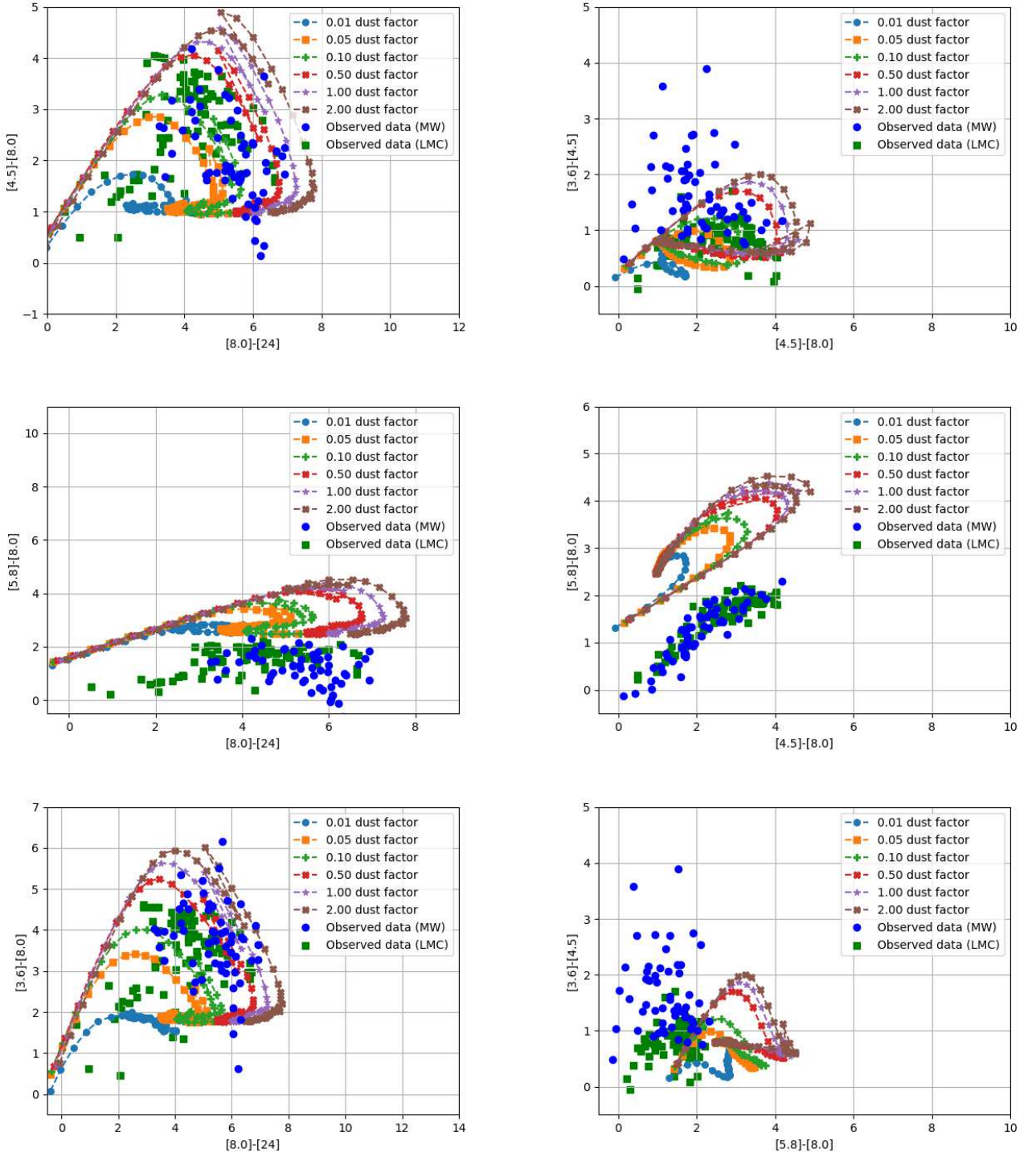


Fig. 3: Impact of the dust abundance variation on the position of evolutionary sequence of modelling results in the color-color diagrams for models of PNe in MW with the carbonates dust grains at $A = 8.0$ and the PN progenitor mass of $1.0M_{\odot}$.

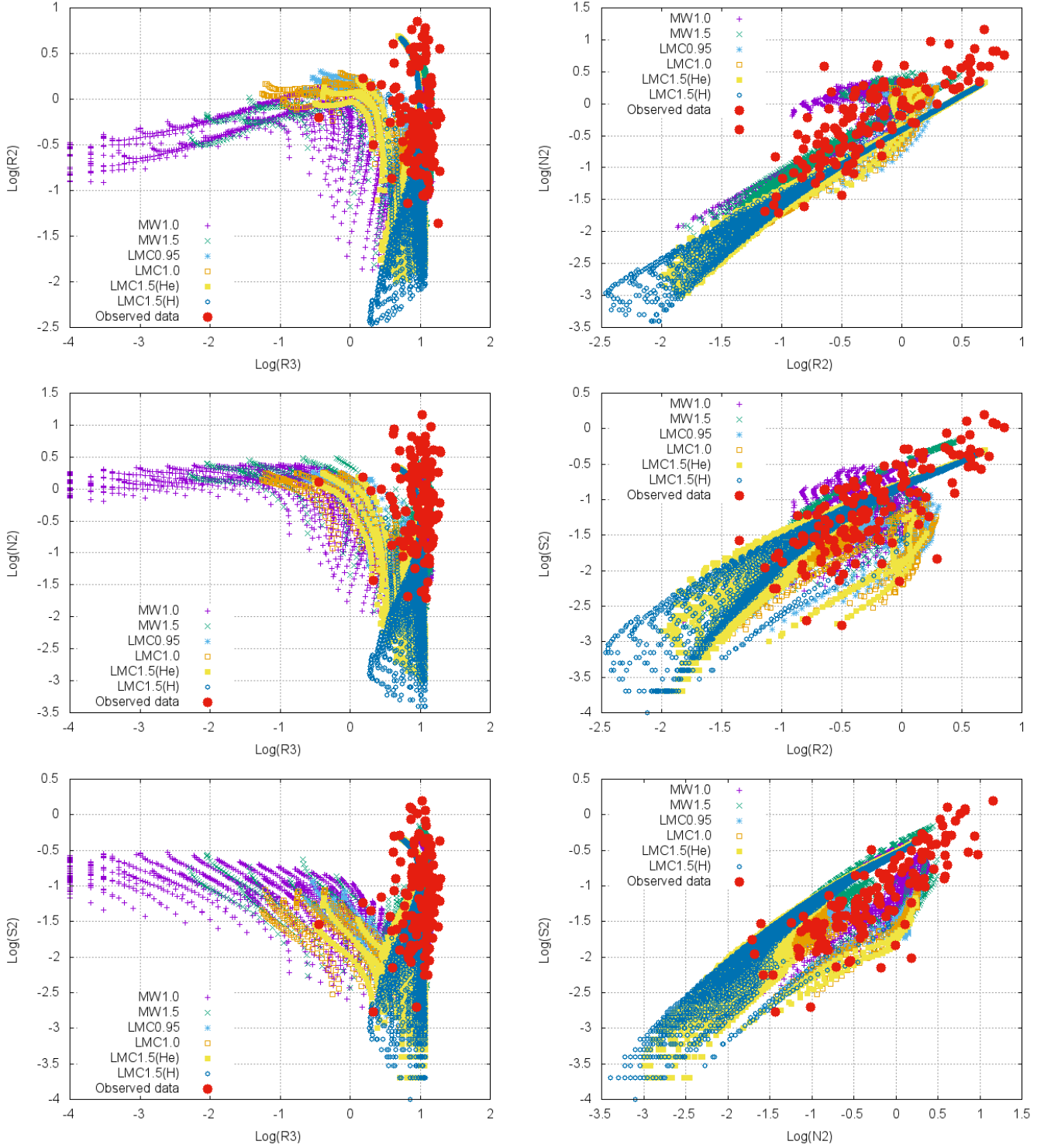


Fig. 4: Comparison of the modelling intensities of the optical strong emission lines, obtained from PhM of PNe in MW and LMC calculated for the progenitor stars of $0.95M_{\odot}$, $1.0M_{\odot}$ and $1.5M_{\odot}$, with the corresponding observed data (see description in the text).