s-Process in low-metallicity stars – I. Theoretical predictions

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ABSTRACT
A large sample of carbon-enhanced metal-poor stars enriched in s-process elements (CEMP-s) have been observed in the Galactic halo. These stars of low mass ($M \sim 0.9 \, M_\odot$) are located on the main-sequence or the red-giant phase, and do not undergo third dredge-up (TDU) episodes. The s-process enhancement is most plausibly due to accretion in a binary system from a more massive companion when on the asymptotic giant branch (AGB) phase (now a white dwarf). In order to interpret the spectroscopic observations, updated AGB models are needed to follow in detail the s-process nucleosynthesis. We present nucleosynthesis calculations based on AGB stellar models obtained with Frascati Raphson-Newton Evolutionary Code (FRANEC) for low initial stellar masses and low metallicities. For a given metallicity, a wide spread in the abundance of the s-process elements is obtained by varying the amount of $^{13}$C and its profile in the pocket, where the $^{13}$C($\alpha$, n)$^{16}$O reaction is the major neutron source, releasing neutrons in radiative conditions during the interpulse phase. We also account for the second neutron source $^{22}$Ne($\alpha$, n)$^{25}$Mg, partially activated during convective thermal pulses. We discuss the surface abundance of elements from carbon to bismuth, for AGB models of initial masses $M = 1.3$–$2 \, M_\odot$, low metallicities ([Fe/H] from $-1$ down to $-3.6$) and for different $^{13}$C-pocket efficiencies. In particular, we analyse the relative behaviour of the three s-process peaks: light-s (Is at magic neutron number $N = 50$), heavy-s (hs at $N = 82$) and lead ($N = 126$). Two s-process indicators, [hs/ls] and [Pb/hs], are needed in order to characterize the s-process distribution. In the on-line material, we provide a set of data tables with surface predictions. Our final objective is to provide a full set of theoretical models of low-mass low-metallicity s-process-enhanced stars. In a forthcoming paper, we will test our results through a comparison with observations of CEMP-s stars.

Key words: nuclear reactions, nucleosynthesis, abundances – stars: carbon – stars: Population II.

1 INTRODUCTION
In the last few years, high-resolution spectroscopic surveys of very metal-poor stars have acquired particular interest, especially for those stars with an appreciable carbon enhancement, i.e. $\text{[C/Fe]} > 1$, the so-called carbon-enhanced metal-poor (CEMP) stars (Beers & Christlieb 2005). A large numbers of CEMP stars have been recently discovered by several survey projects, such as the HK2 objective-prism survey (Beers, Preston & Shectman 1992; Beers et al. 2007), the European Southern Observatory (ESO) Large Programme First Stars with the ESO Very Large Telescope (VLT) and UV–Visual Echelle Spectrograph (UVES) spectrograph (e.g. Cayrel et al. 2004), the Hamburg/ESO survey (Christlieb 2003), the Sloan Extension for Galactic Exploration and Understanding (SEGUE) survey, the SEGUE Stellar Parameter Pipeline (SSPP; Lee et al. 2008a,b), the Sloan Digital Sky Survey (SDSS; York et al. 2000) and the Chemical Abundances of Stars in the Halo (CASH) Project (Roederer et al. 2008). These surveys provide essential means to the understanding of the early Universe and the Galactic chemical evolution.

To interpret the surface abundances of these objects, theoretical stellar evolutionary models are needed. We focus here on CEMP stars with enhancement in elements produced via slow-neutron capture process (s-process; Burbidge et al. 1957; Clayton 1961, 1968;
Käppeler et al. (1982), the so-called CEMP-s stars. It is commonly assumed that CEMP-s stars belong to binary systems where a more massive asymptotic giant branch (AGB) companion, now a white dwarf, had synthesized the s-elements and polluted the observed star by mass transfer. Different studies about AGB nucleosynthesis are available in the literature, either with post-process method or with full stellar evolutionary models (Straniero et al. 1995, 1997, 2003; Goriely & Mowlavi 2000; Herwig 2004; Campbell & Lattanzio 2008; Cristallo et al. 2009a,b). Our calculations are based on Frascati Raphson-Newton Evolutionary Code (FRANEC) (Chieffi & Straniero 1989), coupled with a post-process method which includes a full network up to bismuth (Gallino et al. 1998).

In the late AGB phase, two alternate energy sources are activated, the H-burning shell and the He-burning shell. These two shells are separated by a thin zone in radiative equilibrium, the so-called He-intershell. The H-burning shell progressively erodes the bottom layers of the envelope and produces helium. Consequently, the He-intershell grows in mass and is progressively compressed and heated until the temperature and density become high enough to trigger a thermonuclear runaway in the He shell (thermal pulse, TP). The sudden energy release causes the above layers to be unstable against convection, thus mixing material over the whole He-intershell (Schwarzschild & Härm 1965, 1967). The consequent expansion of the region above the He-burning shell temporarily extinguishes the H-shell. In these conditions, the convective envelope can penetrate under the H-shell, bringing to the surface newly synthesized material (third dredge-up, TDU). During TDU, a chemical discontinuity is established at the interface between the H-rich envelope and the He-intershell, with a sudden change of the opacity, and then, of the temperature gradient. Thus, at the radiative border, the convective velocity becomes abruptly zero, whereas there should exist a transition region, where the convective velocity smoothly decreases to 0. Therefore, a partial mixing may take place. Under this hypothesis, a small amount of hydrogen from the envelope penetrates into the top layers of the He-intershell (Iben & Renzini 1983). Then, at H-shell reignition, a thin 13C-pocket forms in the top layers of the He-intershell, by proton capture on the abundant 12C. There is an upper limit in the 13C production in the pocket. Indeed, a higher proton abundance ingestion would produce 14N by proton capture on 13C. This 13C is primary, because the diffused protons are captured by 13C directly produced by helium burning during previous TPs, regardless of the metallicity. During the interpulse phase, when the temperature in the 13C-pocket increases up to $1 \times 10^8$ K, neutrons are released in radiative conditions via the $^{13}\text{C}(\alpha, n)^{16}\text{O}$ reaction, before the occurrence of the next thermal instability. This reaction constitutes the major neutron source in low-mass AGB stars ($1.2 \lesssim M/M_\odot \lesssim 3$, hereafter LMS), (Straniero et al. 1995; Gallino et al. 1998).

During the convective episode originated by a TP, the s-process material synthesized in the pocket is diluted over the whole He-intershell, while the abundant 14N nuclei in the H ashes are converted to $^{22}\text{Ne}$ via the $^{14}\text{N}(\alpha, \gamma)^{18}\text{F}(\beta^+ + \nu)^{18}\text{O}(\alpha, \gamma)^{22}\text{Ne}$ chain. In LMS, the maximum temperature at the bottom of the TP slightly increases with pulse number, depending on the initial mass and metallicity, reaching $T \approx 3 \times 10^8$ K towards the end of the AGB phase. At this temperature, the $^{22}\text{Ne}(\alpha, n)^{25}\text{Mg}$ reaction is partially activated, producing a neutron burst of small neutron exposure$^3$ but with a high neutron density peak $n_n^{\text{peak}} < 10^{11}$ cm$^{-3}$, followed by a rapid decline (neutron freezeout). The time dependence of this neutron burst is particularly important for defining the freezeout conditions for most of the branchings, that are sensitive to temperature and neutron density. In intermediate-mass AGB stars ($4 \lesssim M/M_\odot \lesssim 8$, hereafter IMS), the maximum temperature during a TP reaches about $3.5 \times 10^8$ K, thus leading to a substantial activation of the $^{22}\text{Ne}(\alpha, n)^{25}\text{Mg}$.

The aim of this paper is to present in detail theoretical predictions of LMS AGB stars ($M = 1.3, 1.4, 1.5$ and $2.0$ $M_\odot$) as a function of metallicity, starting from solar down to $[\text{Fe}/\text{H}] = -3.6$, focusing on stars with $[\text{Fe}/\text{H}] \lesssim -1$. Additional models of IMS in the range of $-1.6 \leq [\text{Fe}/\text{H}] \leq 0$ are discussed to highlight the effects that the mass has on the stellar structure and evolution. Comparison with spectroscopic observations of CEMP-s stars will be presented in a forthcoming paper (Bisterzo et al., in preparation). The models on which we base our calculations are described in Section 2. We study the behaviour of all the elements from carbon to bismuth, the three s-process peaks (light s-process elements ls, heavy s-process elements hs and $[^{56}\text{Fe}]$), and the s-process indicators $[^{20}\text{Ca}]$ and $[^{137}\text{Cs}]$ by varying the metallicity and the $^{13}$C-pocket efficiency, which is a parametrization of the amount of $^{13}$C and its profile in the pocket (Section 3). We also discuss the important effect of $^{26}\text{Ne}$ at low metallicties (Section 4), and the relevance of Na (and Mg) abundances as indicators of the initial AGB mass (Section 5). In Section 6, we give our conclusions.

2 DESCRIPTION OF THE MODELS

We perform the s-process nucleosynthesis with a post-process method (Gallino et al. 1998) based on full evolutionary models obtained with FRANEC code (Straniero et al. 1997, 2000, 2003). Our post-processing calculations follow the convective instabilities generated by TPs, the $^{13}$C-pocket burning and the TDU episodes. The nuclear reaction rates are updated to 2009 (see KADoNiS and further references given in Appendix A) (see on-line material). The main difference with respect to previous publications is the discovery and the correction of an old bug in the models, which affected the treatment of $^{16}\text{O}$ produced in the pocket via $^{13}\text{C}(\alpha, n)^{16}\text{O}$. In addition, protons captures are now included to improve the prediction of the light elements. In particular, $^{13}$F reaction rates of isotopes involving charged particles are taken from the Nuclear Astrophysics Compilation of REAction Rates (NACRE) compilation (Angulo et al. 1999) (web site http://nptpm3.ub.ac.be/Nacre/barre_data_base.htm). We follow the prescriptions given by Straniero et al. (2003) for input data such as

$^3$The metallicity is defined as $[\text{Fe}/\text{H}] = \log_{10}(\text{Fe}/\text{H}) - \log_{10}(\text{Fe}/\text{H})_\odot$. (1)

$^4$We define ls and hs as $[\text{ls}/\text{Fe}] = 1/2([\text{Y}/\text{Fe}] + [\text{Zr}/\text{Fe}])$. (2)

$^5$We exclude Sr from the ls elements and Ba from the hs elements because they are affected by spectroscopic uncertainties, as discussed by Busso et al. (1995) (see also Bisterzo et al., in preparation). Moreover, non-local thermodynamical equilibrium (NLTE) corrections can be significant for Sr and Ba in particular at low metallicties (Andrievsky et al. 2009; Moshonkina et al. 2008; Short & Hauschildt 2006).

$^6$Karlsruhe Astrophysical Data Base of Nucleosynthesis in Stars, web site http://nuclear-astrophysics.fzk.de/kadonis/
(i) the mass of the material dredged up at each TDU episode,
(ii) the temporal history of the temperature and density during the TP and their distribution in the various mass zones of the convective TP,
(iii) the mass of the H-shell,
(iv) the mass of the He-intershell,
(v) the overlapping factor r between successive TDUs,
(vi) the mass of the envelope, which decreases with the TP number because of mass loss and by the activation of the H-burning shell, which progressively erodes the bottom of the envelope.

The interpolation formulae by Straniero et al. (2003) were available in a grid of masses up to $M = 2 \, M_\odot$ and in the metallicity range of $-1 \lesssim [\text{Fe}/\text{H}] \lesssim 0$. We have further extrapolated the stellar parameters down to $[\text{Fe}/\text{H}] = -3.6$.

For a given metallicity, a spread in the $s$-process elements is observed in MS, S, C(N) and Ba stars of the Galactic disc (see Busso et al. 1995, 2001; Abia et al. 2001, 2002; Gallino et al. 2005; Husti & Gallino 2008). At low metallicities, recent high-resolution spectroscopic measurements of CEMP-$s$ stars showed an even larger spread (Ivans et al. 2005; Aoki et al. 2006; Bisterzo & Gallino 2008; Bisterzo et al. 2008; Roederer et al. 2008; Sneden, Cowan & Gallino 2008; Thompson et al. 2008). A range of $s$-process efficiencies is therefore needed in order to interpret the observations.

In our calculations, we artificially introduce the $^{13}$C-pocket, which is treated as a free parameter and kept constant pulse by pulse. Starting from the ST case adopted by Gallino et al. (1998) and Arlandini et al. (1999), which was shown to reproduce the solar $s$-process main component as the average of the 1.5 and 3.0 $M_\odot$ models at half solar metallicity (as described in Appendix A), we multiply or divide the $^{13}$C and ($^{14}$N) abundances in the pocket by different factors. The pocket extends in mass for $9.4 \times 10^{-9} \, M_\odot$ (for LMS about 1/20 of the typical mass involved in a TP), and contains $4.7 \times 10^{-6} \, M_\odot$ of $^{13}$C and $1.6 \times 10^{-7} \, M_\odot$ of $^{14}$N. These masses are the integrated masses in the pocket accounting for the $^{13}$C and $^{14}$N profiles, respectively. $^{14}$N has a resonant neutron capture reaction rate ($\sigma^{14}_N(n, p)^{15}_C(\text{LIANG}) = 1.85 \, \text{mbarn}$; Koehler & O'Brien 1989). $^{14}_N(n, p)^{15}_C$ prevents the captured neutrons to be available for the $s$-process nucleosynthesis (while $^{13}_C$ has a very low neutron capture cross-section). We exclude the possible upper zone close to the border of the TDU where higher proton injection would produce $^{14}_N > ^{13}_C$. The case ST $\times 2$ corresponds to an upper limit, because further proton ingestion leads to the formation of $^{13}$N at expenses of $^{13}$C. The $s$-process efficiency of the $^{13}$C-pocket increases by decreasing the metallicity because of the lower number of iron seeds. We may define a minimum $^{13}$C-pocket as the one which significantly affect the final $s$ distribution, below which the $s$-process path mostly depends on the $^{22}_Ne$ neutron exposure only. As first approximation, for solar metallicity the lowest $^{13}$C-pocket is ST/6, and ST/150 for $[\text{Fe}/\text{H}] = -2.6$ (see Section 3, Fig. 5 for further details). In IMS, the He-intershell mass involved is smaller than LMS by one order of magnitude and the TDU efficiency is reduced. For this reason, a different choice of $^{13}$C-pocket is used for these stars: we defined the case ST-IMS, with $M^{(13}_C\text{ST-IMS}) = 10^{-7} \, M_\odot$.

The crude approximation in the treatment of the $^{13}$C-pocket reflects a significant uncertainty which affects AGB models: in particular, the mixing processes at radiative/convective interfaces during TDU episode. In fact, the penetration of protons in the He-intershell during TDUs is currently a matter of study and one of the most debated issues. Models including rotation (Langer et al. 1999) or gravity waves (Denissenkov & Tout 2003) have obtained a partial mixing zone at the base of the convective envelope during TDU episode, which leads to the formation of a $^{13}$C-rich layer of limited mass extension. Similar results have been obtained by Herwig et al. (1997) and Herwig (2000), who introduced an exponential diffusive overshoot at the borders of all convective zones. A formally similar algorithm, but based on a different mixing scheme (i.e. not diffusive) has been proposed by Straniero, Gallino & Cristallo (2006) (see also Cristallo et al. 2009a). Finally, we remind that the efficiency of the TDU itself is significantly affected by the different treatment of the mixing algorithm, and it is currently a main problem with AGB computations. Different evolutionary codes do not reproduce the same results, since they are based on different treatment of the mixing algorithm (see for instance Straniero et al. 2003; Herwig 2004; Karakas & Lattanzio 2007; Stancliffe & Jeffery 2007; Cristallo et al. 2009a, and references therein).

In AGB stars, photospheric $s$-process enrichment is observed only when the TDU takes place. According to FRANEC model, for LMS it occurs after a limited number of pulses, when the mass of the H-exhausted core reaches $\sim 0.6 \, M_\odot$ (Straniero et al. 2003), bringing freshly synthesized material from the He-intershell into the envelope. The TDU efficiency depends on the envelope mass and on the H-burning rate (see Straniero et al. 2000). The amount of the mass dredged up by each TDU episode, $\delta m_{\text{TDU}}$, first increases as the core mass $m_\text{H}$ increases, and then decreases until vanishing when the envelope mass is reduced by mass loss to a fraction of it (about $0.5 \, M_\odot$ at solar metallicity).

The minimum envelope mass for the occurrence of the TDU depends upon the metallicity, the core mass and the mass loss adopted. The minimum initial mass for a star that undergoes recursive TDU episodes depends on the metallicity. For a solar composition model, $M^{\text{min}}_{\text{TDU}} \sim 1.4 \, M_\odot$, it decreases with metallicity (Straniero et al. 2003). In Fig. 1, we show the mass involved in TDUs (top panel) and the maximum temperature at the base of the convective shell generated by the TPs (bottom panel) as a function of the position in the mass of the H-shell, $m_\text{H}$, for AGB models of solar metallicity and different initial masses. Calculations of $M \leq 2.5 \, M_\odot$ have been computed with interpolation formulae published by Straniero et al. (2003). Note that the mass involved in the TDU increases with the initial AGB mass at $[\text{Fe}/\text{H}] = 0$. At solar metallicity $M = 3 \, M_\odot$ shows a peculiar behaviour of the TDU mass. Indeed, its maximum TDU mass is of the same order of $M = 2.5 \, M_\odot$, and does not further increase. The same of Fig. 1 is shown in Fig. 2, but for $[\text{Fe}/\text{H}] = -0.8$, where the mass involved in the TDU increases. Significant differences are shown for $M = 3 \, M_\odot$ at $[\text{Fe}/\text{H}] = -0.8$, with respect to LMS models: the first TP with TDU occurs when the mass of the H-shell is $m_\text{H} \sim 0.7 \, M_\odot$ (instead of $0.6 \, M_\odot$ as for $M \leq 2.5 \, M_\odot$) and the TDU is less efficient. It was shown by Domínguez et al. (1999) (see also Boothroyd & Sackmann 1988) that, for a given initial mass, the core mass increases by decreasing $[\text{Fe}/\text{H}]$ (Fig. 3). Then, for $[\text{Fe}/\text{H}] < -1.3$, an initial mass $M = 3 \, M_\odot$ approaches the behaviour of IMS stars, characterized by a thinner He-intershell and a weaker TDU. Therefore, $M = 3 \, M_\odot$ behaves as an LMS for disc metallicities and as a IMS for halo metallicities. For $-1.3 \leq [\text{Fe}/\text{H}] \leq -0.8$, we adopt the TDU mass $\delta m_{\text{TDU}}$ shown in Fig. 2 for each initial mass. Then, we assume an increase by a factor of 2 in the metallicity range $-2 < [\text{Fe}/\text{H}] < -1.3$, and a further factor of 2 for $[\text{Fe}/\text{H}] \leq -2$ for AGBs with $M = 1.3, 1.4$ and $1.5 \, M_\odot$. For $M = 2 \, M_\odot$, we adopt an increase of a factor of 2 in all the metallicity range $-3.6 \leq [\text{Fe}/\text{H}] < -1.3$, following detailed results of AGB models (Cristallo et al. 2009a). Indeed, as shown in Fig. 3, $M = 2 \, M_\odot$ at $[\text{Fe}/\text{H}] = -2.3$ is not far from the transition zone between LMS and IMS stars. For initial masses in the range...
of $1.3 \leq M \leq 2.0 \, M_\odot$ and $-3.6 \leq [\text{Fe}/\text{H}] \leq -1.3$, we assumed the values of models with $[\text{Fe}/\text{H}] = -0.8$ for the other input data (like the temperature and density during the TP, the mass of the H-shell and the He-intershell, the overlapping factor and the residual mass of the envelope).

Another debated problem is the evaluation of the mass loss, which plays a key role during the AGB phase. Many stellar properties of the AGB phase depend on the mass loss: for instance, the efficiency of the TDU, the number of pulses and, therefore, the duration of this evolutionary phase. Different methods were developed to estimate the mass-loss rate based on

(i) observations of circumstellar envelope in giants and supergiants (Reimers 1977),

(ii) dynamical calculations for atmospheric Mira-like stars (Bloecker 1995),

(iii) the observed mass-loss period and the period–luminosity relations of AGB stars (Vassiliadis & Wood 1993; recently revised by Straniero et al. 2006 who account for most recent infrared data).

In the models adopted here, the mass loss is estimated with the Reimers formula:

$$\frac{dM}{dt} = -\eta \times (1.34 \times 10^5) \frac{L^2}{M_{\text{eff}}^2} (M_\odot \cdot \text{yr}^{-1}),$$

where $\eta$ is the Reimers parameter; $M, R$ and $L$ are in solar units. We set $\eta = 0.3$ for $M = 1.3-1.5 \, M_\odot$, $\eta = 0.5$ for $M = 2.0 \, M_\odot$, and $\eta = 1$ for $M = 3.0 \, M_\odot$.

With this mass loss, at $[\text{Fe}/\text{H}] = -2.6$, $M = 1.3 \, M_\odot$ shows five TPs followed by TDU, $M = 1.5 \, M_\odot$ experiences 20 TPs with TDU, while $M = 2.0 \, M_\odot$ shows 26 TDUs. The poor knowledge of the actual mass-loss rate remains one of the major uncertainties of AGB stellar models. In particular, observational constraints for the calibration of the mass-loss rate at very low metallicities are lacking (see Straniero et al. 2006). Using the prescription of Reimers, as
compared with the one by Vassiliadis & Wood (1993), few differences in the model results are obtained during the AGB phase, with the exception of the last TPs where superwind takes place (Iben & Renzini 1983). On the other hand, in our models, the TDU episodes cease when the envelope mass is still substantial, and all the superwind phase will take place afterward without further variations in the chemical composition.

IMS AGB models are strongly affected by the mass-loss evaluation (see Straniero et al. 2000; van Loon 2006). For IMS stars, we based our calculations on FRANEC AGB models of $M = 5.0 \, M_\odot$ at $[\text{Fe}/\text{H}] = 0$ and $-1.3$ (Straniero et al. 2000). These two models show very similar characteristics during TP phase, as the maximum temperature at the bottom of the TP (3.6 and $3.7 \times 10^5 \, \text{K}$, respectively), the mass of the AGB almost constant pulse by pulse ($1.2-1.3 \times 10^{-3} \, M_\odot$) and the mass of the He-intershell ($\sim 3 \times 10^{-3} \, M_\odot$). Extrapolating, this might imply that for halo metallicities, the structure of $M = 5.0 \, M_\odot$ is barely distinguishable from solar. Similar characteristics are obtained for a $M = 7 \, M_\odot$ model (Straniero et al. 2000), with the exception of the TDU mass which is reduced by a factor of 6 with respect to $M = 5.0 \, M_\odot$ at $[\text{Fe}/\text{H}] = 0$. With our mass-loss choice, the $M = 5 \, M_\odot$ model experience 24 TPs followed by TDU, leaving a residual total mass of 1.67 $M_\odot$ and a core mass of 0.9 $M_\odot$. Since in IMS the temperatures at the bottom of the convective pulse and the peak neutron density are higher than in LMS ($T_s \sim 3.5; n_s \sim 10^{11} \, \text{cm}^{-3}$), the neutron source $^{22}\text{Ne}(\alpha, n)^{25}\text{Mg}$ is more efficiently activated. Here, neutron-rich isotopes involved in important branchings along the s-process, like $^{88}\text{Kr}, ^{89}\text{Rb}$ and $^{96}\text{Zr}$, are strongly enhanced. As already demonstrated by Travaglio et al. (2004), a remarkable s-process contribution to the isotopes up to zirconium is provided by IMSs during thermally pulsing phases via $^{22}\text{Ne}(\alpha, n)^{25}\text{Mg}$, the main neutron source in these stars. Other mixing and nuclear burning phenomena not treated here are find to occur in IMS, as hot bottom burning (Sugimoto 1971; Iben 1973; Karakas & Lattanzio 2003; Ventura & D’Antona 2005), or, for $[\text{Fe}/\text{H}] \lesssim -2.3$, hot TDU (Goriely & Siess 2004; Herwig 2004; Campbell & Lattanzio 2008; Lau, Stancliffe & Tout 2009). When hot bottom burning occurs (during the interpulse phase), the bottom of the convective envelope reaches the top of the H-burning and the temperature at the base is large enough ($T > 5 \times 10^7 \, \text{K}$) to activate the CNO, NeNa and MgAl cycles of H-burning. The hot TDU, instead, is an extremely efficient dredge-up occurring at low metallicities, in which the envelope reaches almost the bottom of the intershell (or perhaps beyond it, if overshooting is included at low metallicities Herwig 2004; Lau et al. 2009). This last phenomenon modifies the efficiency of the TDU and, then, may influence the structure of the star and its evolution. Nucleosynthesis models which include hot TDU are still a matter for study. For this reason, only IMS AGB models of disc metallicities are discussed here ($M = 5.0$ and $7.0 \, M_\odot$; $-1.6 \leq [\text{Fe}/\text{H}] \leq 0$).

At $[\text{Fe}/\text{H}] \lesssim -2.3$, LMS may experience a single and anomalous TDU episode. It occurs when the convective zone generated by the first fully developed TP extends till the H-rich zone, bringing protons at high temperature and causing the development of a violent thermonuclear runaway (Hollowell, Iben & Fujimoto 1990; Fujimoto, Ikeda & Iben 2000; Iwamoto et al. 2004; Campbell & Lattanzio 2008; Cristallo et al. 2009b; Lau et al. 2009). In the present calculations, we do not consider such an extreme case.

### 2.1 Initial chemical composition

The initial compositions (in mass fractions) used for He are: $Y = 0.28$ for $-0.3 \leq [\text{Fe}/\text{H}] \leq 0.0; Y = 0.27$ for $-0.8 \leq [\text{Fe}/\text{H}] < -0.3$; $Y = 0.26$ for $-1.3 \leq [\text{Fe}/\text{H}] < -0.8; Y = 0.25$ for $[\text{Fe}/\text{H}] < -1.3$.

The initial isotopic composition of the other isotopes is based on the solar meteoritic values of Anders & Grevesse (1989), except for C, N and O isotopes, which are upgraded to that of Lodders (2003). For metallicity lower than solar, we use solar scaled abundances, with the exception of the $\alpha$ elements. For oxygen, we assumed a linear increase $[\text{O}/\text{Fe}]$ with decreasing $[\text{Fe}/\text{H}]$ (Abia et al. 2001). $[\text{O}/\text{Fe}] = -0.4$ [\text{Fe}/\text{H}]. For the other $\alpha$ elements ($^{20}\text{Ne}, ^{24}\text{Mg}, ^{32}\text{S}, ^{28}\text{Si}$, $^{56}\text{Fe}, ^{40}\text{Ca}, ^{48}\text{Ti}$), we adopt a linear relation $[\alpha/\text{Fe}] = -0.3 [\text{Fe}/\text{H}]$ at disc metallicities ($-1 \leq [\text{Fe}/\text{H}] \leq 0$), and an average constant $[\alpha/\text{Fe}] = 0.3$ dex for $[\text{Fe}/\text{H}] \leq -1$, following the trend observed in unevolved stars (Cayrel et al. 2004; François et al. 2004).

We took into account the effect of the first dredge-up (Busso, Gallino & Wasserburg 1999) and second dredge-up (SDU occurring in IMS; Lattanzio et al. 1996; Busso et al. 1999) in the initial C, N, O composition of our AGB models. Concerning nitrogen, we assumed an initial value after the first dredge-up $[\text{N}/\text{Fe}] = 0.3 -0.4$, depending on the mass of the AGB, as predicted by full evolutionary models by Cristallo et al. (2009a,b). The $[\text{N}/\text{Fe}]$ surface prediction increases with the TDU number owing to dredging-up to the surface also the ashes of the temporary inactivated H-burning shell, where all CNO isotopes are almost converted to $^{14}\text{N}$, including the primary $^{12}\text{C}$ that is present in the envelope due to previous TDU episodes. As a consequence, $[\text{N}/\text{Fe}]$ increases with the number of TDU episodes.

### 3 RESULTS AND DISCUSSION

#### 3.1 The three s-process peaks

Nuclei with a magic neutron number ($N = 50, 82$ and 126) are essentially produced by the s-process, since their low neutron capture cross-sections act as a bottleneck for the s-path.

In Fig. 4, we have shown the envelope abundances after each TDU for an AGB model of initial mass $M = 1.5 \, M_\odot$, a case ST and $[\text{Fe}/\text{H}] = -2.6$ (top panel). As a comparison, we plot the envelope abundances for the same case, but at $[\text{Fe}/\text{H}] = 0$ (bottom panel). We underline the completely different shapes of the two distributions. At low metallicities, the distribution is shifted towards heavier elements: in particular, already after the first TDU, lead receives an extraordinary contribution ($^{209}\text{Pb}/^{207}\text{Pb} \sim 4.1$), producing also a huge amount of $^{208}\text{Bi}$ by neutron captures on $^{208}\text{Pb}$ ($^{208}\text{Bi}/^{207}\text{Bi} \sim 3.9$). This occurs because $^{40}\text{Ar}$ (the seed of the s-process) decreases with metallicity, thus the number of neutrons available per iron seed increases, due to the fact that the $^{12}\text{C}$ neutron source is primary (Clayton 1988). Hence, the neutron fluence overcomes the first two peaks, directly feeding $^{208}\text{Pb}$ (Gallino et al. 1998; Goriely & Mowlavi 2000; Travaglio et al. 2001). Note that the increase of heavy elements is more pronounced during the first TPs, achieving an asymptotic trend beyond the 10th TDU.

During the TDU, the material of the H-shell is carried to the surface: this zone is rich of primary $^{14}\text{N}$ produced from primary $^{12}\text{C}$ during the CNO cycle. The nitrogen surface prediction takes into account for this primary $^{14}\text{N}$, and, therefore, $[\text{N}/\text{Fe}]$ increases with the number of TDU episodes and by decreasing the metallicity. Carbon is efficiently enhanced in the envelope at $[\text{Fe}/\text{H}] = -2.6$ already at the first TDUs (for the case ST, we predict $[\text{C}/\text{Fe}]$; Fig. 4, top panel). The overproduction of carbon, in fact, increases by decreasing the metallicity due to the primary amount of $^{12}\text{C}$ and to the deeper TDUs as well (Section 2). Two further peaks are predicted: at Sn (before hs) and at Hf/W (before Pb/Bi). These elements receive an s-process contribution to the solar abundances.
Figure 4. Top panel: elemental composition in the envelope after different TDU episodes (labelled as \( n(i) \)), for an AGB model of initial mass \( M = 1.5 \, M_\odot \), initial metallicity \([\text{Fe/H}] = -2.6\) and standard choice of the \(^{13}\text{C}\)-pocket (case ST; Gallino et al. 1998). The label ‘n0’ stands for the initial composition. Note that after 15 TPs, the abundances \([\text{El/Fe}]\) reach an asymptotic value (the label ‘El’ stands for a generic element). The initial \( \text{Cr} \) and \( \text{Mn} \) abundances are chosen in agreement with the observations of unevolved halo stars (Cayrel et al. 2004; François et al. 2004). The assumed value \([\text{Mn/Fe}] = -0.4\) may increase up to \([\text{Mn/Fe}] \sim -0.1\) due to NLTE corrections (Bergemann & Gehren 2008). Bottom panel: for comparison, we report the similar case for a model with the same initial mass, but at \([\text{Fe/H}] = 0\). These models are for intrinsic AGBs (\([\text{Zr/Nb}] \sim 1\), see Section 3.2). Note the difference of scale between the two plots.

of \( \text{Sn}_s = 66 \) per cent, \( \text{Hf}_s = 59 \) per cent, \( \text{Ta}_s = 45 \) per cent, \( \text{W}_s = 64 \) per cent (see Appendix A).

Fig. 5 (top panel) shows AGB models of \( M = 1.5 \, M_\odot \) at \([\text{Fe/H}] = -2.6\), by varying the efficiency of the \(^{13}\text{C}\)-pocket. Similarly, we show in Fig. 5 (bottom panel) the same result at solar metallicity. The solid heavy line represents the case ST. Decreasing the \(^{13}\text{C}\)-pocket efficiency to ST/24, lead is reduced of more than 1 dex with respect to the ST case. At \([\text{Fe/H}] = -2.6\), for \(^{13}\text{C}\)-pockets \( \leq \text{ST/75} \), the \(^{13}\text{C}\) is negligible and the \( s \)-process production is principally due to the \(^{22}\text{Ne}(\alpha, n)^{25}\text{Mg}\) reaction activated during the TPs. Some production of the \( ls \) elements is still observed with a case ST/150.

In Table 1, we list the theoretical predictions for elements from \( \text{Sr} \) to \( \text{Bi} \) at the last TDU for an initial mass \( M = 1.5 \, M_\odot \) at \([\text{Fe/H}] = -2.6\) and different \(^{13}\text{C}\)-pocket efficiencies (ST, ST/12, ST/45, ST/75). In Columns 3 to 6, we have shown the \([\text{El/Fe}]\) predictions, which, in Columns 7 to 10, are normalized to europium in logarithmic scale \([\text{El/Eu}]\) (the label ‘El’ stands for a generic element). The case ST predicts \([\text{hs/ls}] = 0.6\) (Column 3), while \([\text{hs/ls}] \) reaches \( -0.25 \) by decreasing the \( s \)-process efficiency down to \( \sim \text{ST/70} \) (similar to the case ST at \([\text{Fe/H}] = -0.3\), see Appendix A). Since europium is an element with dominating \( r \)-process abundances, the lanthanum/europium ratio provides a measure of the \( s \)- and \( r \)-process components in halo stars. A pure \( s \)-process contribution predicts \( 0.8 \leq [\text{La/Eu}] \leq 1.1 \) at \([\text{Fe/H}] = -2.6\) (Columns 7 to 10). Values \([\text{La/Eu}] \lesssim 0.4\) indicate stars that have experienced an important \( r \)-process contribution in addition to the \( s \)-process enhancements (see Bisterzo et al., in preparation).
Another parameter affecting the overabundances is the initial AGB mass, which determines not only the \(s\)-process element abundances, but also some of the light element abundances (like Na and Mg), which are not affected by the \(^{13}\text{C}\)-pocket efficiency (see Section 5 for a detailed description). In Fig. 6, we show a comparison of the theoretical results obtained for \(1.2 \leq M/M_\odot \leq 2.0\). The limited number of TDUs for the lowest mass models explains the smaller abundances. Changing the initial mass, we predict variations up to 2.5 dex for the light elements (as Na and Mg, as discussed in Section 5), 1.5 dex for the hs peak, about 2 dex for the ls peak and 1.5 dex for Pb. In Appendix B (see on-line material (Section B1)), we list surface elemental predictions at [Fe/H] = −2.6 for different initial AGB masses: \(M_{\text{AGB}}\) ini = 1.3, 1.4, 1.5 and 2.0 \(M_\odot\).

In order to extend our theoretical analysis to different stellar populations, we discuss the AGB results by varying the metallicity. In Figs 7 to 9, we present theoretical predictions of [ls/Fe], [hs/Fe] and [Pb/Fe] versus [Fe/H] for AGB models with initial masses \(M = 1.3, 1.5\) and 2.0 \(M_\odot\) and different \(^{13}\text{C}\)-pocket efficiencies (from ST \(\times 2\) down to ST/150). In Appendix B (Section B2), we give tabulated surface predictions for AGB initial masses \(M = 1.3\) and 1.5 \(M_\odot\), \(-3.6 \leq [\text{Fe/H}] \leq -1.0\) and two choices of the \(^{13}\text{C}\)-pocket (ST and ST/12). Obviously, models with more TDU (Figs 1 and 2) show larger surface \(s\)-process enhancements. In Table 2, we list the number of pulses with TDU experienced by each model. Results from 1.5 and 2 \(M_\odot\) models are in general quite similar (Fig. 7, middle and bottom panels). Depending on the metal content and on the efficiency of the \(^{13}\text{C}\)-pocket, the behaviour of the [ls/Fe] peak is highly non-linear as a function of the metallicity and on the \(^{13}\text{C}\) amount. For example, in the ST case of the \(M = 1.5 M_\odot\) model, the [ls/Fe] ratio increases starting from solar down to [Fe/H] \(-0.8\), where there is a local maximum. Then, [ls/Fe]
Table 1. Theoretical predictions of [El/Fe] and [El/Eu] for elements from Sr to Bi (the label ‘El’ stands for a generic element), at [Fe/H] = −2.6, for $M = 1.5 \, M_{\odot}$ models and various choices of the $^{13}$C-pocket (ST, ST/12, ST/45, ST/75).

| El | Z  | ST   | ST/12 | [El/Fe] ST/45 | ST/75 | ST   | ST/12 | ST/45 | ST/75 |
|----|----|------|-------|--------------|-------|------|-------|-------|-------|
|    | (1) | (2)  | (3)   | (4)          | (5)   | (6)  | (7)   | (8)   | (9)   |
| Sr | 38 | 1.42 | 2.25 | 2.00 | 1.81 | 0.16 | 0.53 | 0.92 | 1.36 |
| Y  | 39 | 1.46 | 2.41 | 2.08 | 1.85 | 0.20 | 0.69 | 1.00 | 1.40 |
| Zr | 40 | 1.45 | 2.45 | 2.02 | 1.76 | 0.19 | 0.73 | 0.94 | 1.31 |
| Nb | 41 | 1.47 | 2.49 | 2.05 | 1.78 | 0.21 | 0.77 | 0.97 | 1.33 |
| Mo | 42 | 1.75 | 2.33 | 2.15 | 1.55 | 0.07 | 0.61 | 0.77 | 1.10 |
| Ru | 44 | 1.07 | 2.06 | 1.56 | 1.27 | −0.19 | 0.34 | 0.48 | 0.82 |
| Rh | 45 | 0.71 | 1.67 | 1.19 | 0.92 | −0.55 | −0.05 | 0.11 | 0.48 |
| Pd | 46 | 1.08 | 2.07 | 1.63 | 1.35 | −0.18 | 0.35 | 0.55 | 0.90 |
| Ag | 47 | 0.72 | 1.68 | 1.26 | 1.00 | −0.54 | −0.04 | 0.18 | 0.55 |
| Cd | 48 | 1.18 | 2.16 | 1.76 | 1.47 | −0.08 | 0.44 | 0.68 | 1.02 |
| In | 49 | 1.01 | 1.96 | 1.56 | 1.27 | −0.25 | 0.24 | 0.48 | 0.82 |
| Sn | 50 | 1.42 | 2.36 | 1.87 | 1.54 | 0.16 | 0.64 | 0.79 | 1.09 |
| Sb | 51 | 1.11 | 2.02 | 1.51 | 1.17 | −0.15 | 0.30 | 0.43 | 0.72 |
| Te | 52 | 0.99 | 1.88 | 1.37 | 1.03 | −0.27 | 0.16 | 0.29 | 0.58 |
| I  | 53 | 0.55 | 1.37 | 0.88 | 0.57 | −0.71 | −0.35 | −0.20 | 0.13 |
| Xe | 54 | 1.09 | 1.95 | 1.43 | 1.06 | −0.17 | 0.23 | 0.35 | 0.61 |
| Cs | 55 | 0.91 | 1.77 | 1.29 | 0.92 | −0.35 | 0.05 | 0.21 | 0.48 |
| Ba | 56 | 2.03 | 2.73 | 2.17 | 1.63 | 0.77 | 1.01 | 1.09 | 1.18 |
| La | 57 | 2.06 | 2.69 | 2.12 | 1.52 | 0.80 | 0.97 | 1.04 | 1.07 |
| Ce | 58 | 2.23 | 2.77 | 2.16 | 1.47 | 0.97 | 1.05 | 1.08 | 1.02 |
| Pr | 59 | 2.01 | 2.55 | 1.96 | 1.27 | 0.75 | 0.83 | 0.88 | 0.82 |
| Nd | 60 | 2.11 | 2.62 | 2.00 | 1.28 | 0.85 | 0.90 | 0.92 | 0.83 |
| Sm | 62 | 1.96 | 2.44 | 1.79 | 1.06 | 0.70 | 0.72 | 0.71 | 0.61 |
| Eu | 63 | 1.26 | 1.72 | 1.08 | 0.45 | 0.00 | 0.00 | 0.00 | 0.00 |
| Gd | 64 | 1.68 | 2.16 | 1.49 | 0.79 | 0.42 | 0.44 | 0.41 | 0.34 |
| Tb | 65 | 1.44 | 1.91 | 1.25 | 0.57 | 0.18 | 0.19 | 0.17 | 0.13 |
| Dy | 66 | 1.68 | 2.14 | 1.46 | 0.76 | 0.42 | 0.42 | 0.38 | 0.31 |
| Ho | 67 | 1.44 | 1.89 | 1.21 | 0.55 | 0.18 | 0.17 | 0.13 | 0.10 |
| Er | 68 | 1.81 | 2.26 | 1.57 | 0.85 | 0.55 | 0.54 | 0.49 | 0.41 |
| Tm | 69 | 1.67 | 2.11 | 1.42 | 0.72 | 0.41 | 0.39 | 0.34 | 0.27 |
| Yb | 70 | 2.15 | 2.58 | 1.87 | 1.13 | 0.89 | 0.86 | 0.79 | 0.68 |
| Lu | 71 | 1.87 | 2.28 | 1.58 | 0.85 | 0.61 | 0.56 | 0.50 | 0.41 |
| Hf | 72 | 2.33 | 2.75 | 2.05 | 1.28 | 1.07 | 1.03 | 0.97 | 0.83 |
| Ta | 73 | 2.21 | 2.62 | 1.92 | 1.16 | 0.95 | 0.90 | 0.84 | 0.71 |
| W  | 74 | 2.33 | 2.75 | 2.05 | 1.27 | 1.07 | 1.03 | 0.97 | 0.82 |
| Re | 75 | 1.77 | 2.13 | 1.41 | 0.70 | 0.51 | 0.41 | 0.33 | 0.25 |
| Os | 76 | 1.64 | 2.04 | 1.35 | 0.63 | 0.38 | 0.32 | 0.27 | 0.18 |
| Ir | 77 | 0.82 | 1.19 | 0.56 | 0.09 | −0.44 | −0.53 | −0.52 | −0.35 |
| Pt | 78 | 1.41 | 1.80 | 1.11 | 0.43 | 0.15 | 0.08 | 0.03 | −0.02 |
| Au | 79 | 1.38 | 1.76 | 1.07 | 0.40 | 0.12 | 0.04 | −0.01 | −0.05 |
| Hg | 80 | 2.40 | 2.77 | 2.05 | 1.26 | 1.14 | 1.05 | 0.97 | 0.81 |
| Tl | 81 | 2.46 | 2.72 | 1.93 | 1.16 | 1.20 | 1.00 | 0.85 | 0.71 |
| Pb | 82 | 4.07 | 3.26 | 1.98 | 1.12 | 2.81 | 1.54 | 0.90 | 0.67 |
| Bi | 83 | 3.93 | 2.96 | 1.45 | 0.58 | 2.67 | 1.24 | 0.37 | 0.13 |

[hs/ls] 0.59 0.15 −0.08 −0.52
[Ps/hs] 2.03 0.68 0.01 −0.17

decreases down to [Fe/H] ~ −1.5, because the s-path overcomes the ls (and hs) elements feeding lead. Further decreasing the metallicity ([Fe/H] < −1.5), [ls/ls] reaches a local maximum, the ls nuclei are

efficients $^{13}$C-pockets, e.g. the case ST/12, the highest [ls/ls] value is shifted towards lower metallicities ([Fe/H] ~ −2), because of the lower number of neutrons produced. For [Fe/H] ≤ −2, a flat behaviour is achieved.

The [hs/ls] trend is similar to the behaviour previously discussed for [ls/ls], but with slightly different slopes (Fig. 8). As for [ls/ls], a primary $^{22}$Ne contribution to [hs/ls] is observed for [Fe/H] ≤ −2. When the hs-peak reaches a local maximum, the hs nuclei are used for the production of lead.
[\text{Pb}/\text{Fe}] increases by decreasing the metallicity, covering a range of four orders of magnitude (Fig. 9). [\text{Pb}/\text{Fe}] increases as the AGB initial mass increases, according to the rising number of TPs.

The differences between models presented here and previous publications (Bisterzo et al. 2009; Sneden et al. 2008) are principally due to the correction of a past bug in the code, where we did not account for the poisoning effect of $^{16}\text{O}$ in the pocket produced by the $^{13}\text{C} (\alpha, n)^{16}\text{O}$ reaction. While no variations in the $s$-process abundances are found from solar metallicity down to $[\text{Fe}/\text{H}] = -1.6$, at halo metallicities, the $s$-process abundances may be strongly reduced for high $^{13}\text{C}$-pocket efficiencies. For cases ST $\times$ 2 down to ST, variations up to 0.5 dex are obtained for $M = 1.5$ and 2 M$_{\odot}$. Even higher variations (up to 0.8 dex) are obtained for AGB models of $M = 1.3$ and 1.4 M$_{\odot}$. Changes lower than 0.1 dex are observed for cases <ST/1.5.

The addition of proton captures in the network does not involve variations in the production of $s$-process elements. However, proton captures have a key role in improving the prediction of fluorine (Section 5).

3.2 Nb and Zr predictions and their significance

An intrinsic AGB is a star with high luminosity and low log $g$ that lies on the TP-AGB or post-AGB phase. An extrinsic AGB is located on the main-sequence or on the red-giant branch. In this case, which is the case for CEMP-$s$ stars, the $s$-process abundances are due to mass transfer from a more massive AGB companion, which now is cooling along the white dwarf sequence (Wallerstein & Dominy 1988). These two classes can be discerned by studying the abundances of two elements: Tc and Nb. Long-lived isotopes fed by the $s$-process, like $^{99}\text{Tc}$ ($t_{1/2} = 2 \times 10^5$ yr), can be observed in the intrinsic AGB stars, as first discovered by Merrill (1952). As the interpulse phase in LMS has a typical period of the order of $10^4$ yr, $^{99}\text{Tc}$, brought into the surface after the TDU, does not have time to completely decay. Spectroscopic observations of disc metallicity stars were done in the past for MS, S, C(N) stars, in order to search for intrinsic AGBs by detecting Tc lines (Smith & Lambert 1988, 1990; Brown et al. 1990; Busso et al. 2001; Abia et al. 2002).

Another key element to discriminate between intrinsic and extrinsic AGB stars is niobium. According to Arlandini et al. (1999), solar Nb ($^{93}\text{Nb}$), which is bypassed by the $s$-process fluence, receives a contribution of 85 per cent from the $s$-process (see also Appendix A) by radiogenic decay of $^{93}\text{Zr}$ ($t_{1/2} = 1.5$ Myr). This latter isotope is strongly fed by the $s$-process because of its low neutron caption cross-section (Bao et al. 2000). The long-lived isotope $^{93}\text{Zr}$ partially decays into $^{90}\text{Nb}$ during the interpulse phase and, at each TDU, newly synthesized $^{93}\text{Zr}$ is mixed within the envelope. In intrinsic AGB stars, a fraction of Nb is produced in the envelope by the decay of $^{93}\text{Zr}$. Instead, for extrinsic AGBs, all the $^{93}\text{Zr}$ produced by the $s$-process already decayed into $^{93}\text{Nb}$. Then, for an intrinsic AGB, such as CEMP-$s$ stars, we expect $[\text{Zr}/\text{Nb}] \sim 0$ (dashed line of Fig. 10), while for an extrinsic AGB $[\text{Zr}/\text{Nb}] \sim 0$ (solid line of Fig. 10).

3.3 Intrinsic $s$-process indexes

As demonstrated in Section 3.1, in AGB stars $s$-rich material coming from the He-intershell is mixed with the AGB envelope during each TDU and thus $[\text{ls}/\text{Fe}]$, $[\text{hs}/\text{Fe}]$ and $[\text{Pb}/\text{Fe}]$ increase with the number of TDUs. The elemental distribution after each TDU represents therefore the surface composition of the star.

Instead, in extrinsic AGBs, we do not observe the pristine amount of material synthesized since this material may undergo further mixing with the envelope of the extrinsic AGB star. Low-mass main-sequence stars have a very thin convective envelope. In this case, thermohaline mixing or gravitational settling could dilute the original AGB material (Vauclair 2004; Eggleton, Dearborn & Lattanzio 2006; Charbonnel & Zahn 2007; Denissenkov & Pinsonneault 2008; Stancliffe & Glebbeek 2008; Denissenkov, Pinsonneault & MacGregor 2009). Red giants instead have extended convective envelopes in which the original AGB material is diluted. The dilution factor of the AGB material can be

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Figure 6. Elemental composition in the envelope at the last TDU, for AGB models of initial metallicity $[\text{Fe}/\text{H}] = -2.6$, but different initial masses: $1.2 \leq M/M_{\odot} \leq 2.0$ (cases ST).

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[Diagram showing elemental composition]
Figure 7. Theoretical results of [ls/Fe] versus metallicity, for AGB models of initial mass $M = 1.3 M_\odot$ (top panel), $M = 1.5 M_\odot$ (middle panel) and $M = 2.0 M_\odot$ (bottom panel). A wide range of $^{13}$C-pocket efficiencies is presented. A $1.3 M_\odot$ model undergoes TDU episodes starting from [Fe/H] $\leq -0.6$ (see Figs 2 and 3 of Straniero et al. 2003).

calculated using the formula:

$$[\text{El}^{\text{obs}}/\text{Fe}] = \log(10^{[\text{El}^{\text{AGB}}/\text{Fe}]-\text{dil}} + 10^{[\text{El}^{\star}/\text{Fe}](1 - 10^{-\text{dil}})}),$$ (5)

7This equation is obtained starting from the simple hypothesis that

$$\text{EI}^{\text{obs}} \cdot M^{\text{AGB}} = \text{EI}^{\text{env}} \cdot \Delta M^{\text{AGB}} + \text{EI}^{\text{env}} \cdot M^{\star},$$

where $\text{EI}^{\text{obs}}$ is the mass fraction of the element 'El' observed in the extrinsic star, $\text{EI}^{\text{AGB}}$ is the mass fraction of the element 'El' in the material transferred from the AGB to the companion, $\Delta M^{\text{AGB}}$ is the mass fraction of the element 'El' in the envelope of the observed star before the mass transfer, $M^{\text{obs}}$ is the envelope mass of the observed star, $\Delta M^{\text{AGB}}$ is the material transferred from the AGB to the companion and $M^{\star}$ is the envelope mass of the observed star before the mass transfer.

Figure 8. The same as in Fig. 7, but for [hs/Fe].

where $[\text{El}/\text{Fe}]^{\text{obs}}$ is the overabundance measured in the extrinsic star, $[\text{El}/\text{Fe}]^{\text{AGB}}$ is the amount of the element 'El' in the AGB envelope. The dilution $\text{dil}$, chosen for each star in order to obtain a best fit of the experimental data, is defined as the mass of the convective envelope of the observed star ($M^{\star}$) over the material transferred from the AGB to the companion ($\Delta M^{\text{AGB}}$):

$$\text{dil} = \log \left( \frac{M^{\star}}{\Delta M^{\text{AGB}}} \right).$$ (6)

In this context, the [hs/ls] and [Pb/ls] ratios are extremely valuable indexes for the $s$-process as they are independent of both the TDU efficiency in the AGB star and the dilution of the AGB material on to the companion. Moreover, the [hs/ls] ratio may give a constrain on the initial AGB mass because, with increasing the mass (and decreasing the metallicity), the elements of the first $s$-peak receive a significant contribution from the $^{22}\text{Ne}$(α, n)$^{25}\text{Mg}$ neutron.
source during the convective TP. In Table 3, we list the values of the intrinsic index [hs/ls] at [Fe/H] = −2.6 by changing the \(^{13}\)C-pocket for various AGB initial masses. The [hs/ls] ratio may give a constraint on the initial mass, and it can be an indicator of the \(s\)-process efficiency as well. For example, by comparing \(M = 1.3\) and \(1.5\) \(M_\odot\), the case ST/12 predicts [hs/ls] \(\sim 1.0\) and \(\sim 0.2\) dex, respectively. In Fig. 11, we show the [hs/ls] theoretical predictions versus metallicity for AGB models of \(M = 1.3, 1.5\) and \(2.0\) \(M_\odot\).

While in disc metallicity stars ([Fe/H] \(> -1.5\)), the ratio [hs/ls] provides strong constraints on the mass and on the \(^{13}\)C-pocket efficiency, at low metallicities ([Fe/H] \(\leq -1.5\)) models characterized by the same [hs/ls] value could show different [Pb/Fe] values. For example, for a \(M = 1.3\) \(M_\odot\) model at [Fe/H] = −2.5, the ST/3 and ST/30 cases predict the same [hs/ls] \(\sim 0.5\), while they have [Pb/Fe] \(\sim 3.2\) and 2.4, respectively (see Figs 9 and 11, top panels). Another \(s\)-process indicator is therefore required to discern between different theoretical models: [Pb/hs] (or [Pb/ls]), (Van Eck et al. 2003; Delaude et al. 2004). In Fig. 12, theoretical predictions of [Pb/hs] versus metallicity are shown for different \(^{13}\)C-pockets and different masses (\(M = 1.3, 1.5\) and \(2.0\) \(M_\odot\)). These values are also listed in Table 3 at [Fe/H] = −2.6. [Pb/hs] ratio covers a large spread (0 \(<\) [Pb/hs] \(\lesssim 2\); Fig. 12). The maximum amount of \(^{13}\)C and \(^{14}\)N in the pocket and different hydrogen profiles (then the amount of \(^{13}\)C and \(^{14}\)N in the tails of the pocket) modify the final \(s\)-process distribution. This explains possible differences between the range of [hs/ls] and [Pb/hs] predicted by our models and other results presented in the literature (see Bisterzo et al., in preparation).

In Figs C2 and C3 (Appendix C, on-line material), we show [ls/Fe], [hs/Fe], [Pb/Fe] and [hs/ls] and [Pb/hs] for \(M = 3\) \(M_\odot\) in the metallicity range of −1.6 \(\leq\) [Fe/H] \(\leq 0\). Note that the range of \(^{13}\)C-pockets adopted has a negligible influence on the [ls/Fe] ratio (\(\sim 0.3\) dex). As expected, lead is more sensible to the \(^{13}\)C-pocket efficiency, showing, however, a reduced spread with respect to lower stellar masses (Fig. C2, bottom panel; Appendix C, online material). For \(M = 3\) \(M_\odot\), a behaviour similar to IMS stars is expected for halo metallicities (see Section 2, Fig. 3). We show in

![Figure 9](image)

**Figure 9.** The same as in Fig. 7, but for [Pb/Fe].

![Figure 10](image)

**Figure 10.** Theoretical predictions for [Zr/Fe] and [Nb/Fe] in an extrinsic (solid line) and an intrinsic (dashed line) AGB, with initial mass \(M = 1.5\) \(M_\odot\), and [Fe/H] = −2.6. The efficiency of the \(^{13}\)C-pocket has been set to the ST case.

and 1.5 \(M_\odot\), the case ST/12 predicts [hs/ls] \(\sim 1.0\) and \(\sim 0.2\) dex, respectively. In Fig. 11, we show the [hs/ls] theoretical predictions versus metallicity for AGB models of \(M = 1.3, 1.5\) and \(2.0\) \(M_\odot\).

Table 2. We listed the number of pulses with TDU experienced by each model.

| Stellar mass (\(M_\odot\)) | [Fe/H] | Number of TDUs | [Fe/H] | Number of TDUs |
|--------------------------|--------|---------------|--------|---------------|
| 1.3                      | 0; −0.3| 0             | From −0.5 down to −3.6 | 5             |
| 1.5                      | 0; −0.3| 19            | From −0.5 down to −3.6 | 10            |
| 2.0                      | 0; −0.3| 22, 25        | From −0.5 down to −3.6 | 26            |
| 3.0                      | 0; −0.3| 25            | −0.5; from −0.8 down to −1.6 | 26, 35   |
| 5.0                      | 0; −0.3| 24            | From −0.5 down to −1.6 | 24            |
| 7.0                      | 0; −0.3| 24            | From −0.5 down to −1.6 | 24            |
4 THE IMPORTANCE OF THE PRIMARY $^{22}$Ne AT LOW METALLICITIES

At very low metallicities, a primary production of $^{22}$Ne, which increases with the initial mass, results in the advanced pulses by the conversion of primary $^{12}$C to primary $^{14}$N in the H-burning ashes, via $^{14}$N$(\alpha, \gamma)^{18}$F$(\beta^+ \nu)^{19}$O and $^{16}$O$(\alpha, \gamma)^{22}$Ne reaction during TPs (Mowlavi 1999; Gallino et al. 2006; Husty et al. 2007). The production of primary $^{22}$Ne is more efficient at lower metallicities because a larger abundance of primary $^{12}$C is mixed with the envelope at each TDU episode. The subsequent activation of the H-shell converts almost all CNO nuclei into $^{14}$N. This amount of primary $^{14}$N is left in the H-burning ashes and during the subsequent TP this is converted into primary $^{22}$Ne.

To test the effect of neutron captures on $^{22}$Ne, we show in Fig. 13, the theoretical prediction for AGB models of $M = 1.5 \, M_\odot$ and $[\text{Fe/H}] = -2.6$, without $^{13}$C-pocket (case ST = 0, top panel) and with a case ST (bottom panel). Solid lines represent the ordinary cases, while the dashed lines correspond to cases with the cross-section of $^{22}$Ne($n, \gamma)^{23}$Ne set to zero. Concerning light elements, this test mainly affects $^{23}$Na, which decreases more than 2 dex, thus highlighting the primary production of $^{23}$Na via $^{22}$Ne($n, \gamma)$Ne. For $Z \geq 30$, the larger amount of available neutrons feeds the production of the elements up to lead (blue dotted lines). This makes $^{22}$Ne, as well as $^{23}$Na, the main neutron poison at low metallicity during the $^{22}$Ne neutron burst. As illustrated in Fig. 13 (bottom panel), for a ST case of $s$-process efficiency, $^{22}$Ne remains the most efficient neutron poison even inside the $^{13}$C-pocket during the interpulse

### Table 3

| Mass     | $^{13}$C-pocket | ST/9 | ST/12 | ST/18 | ST/24 | ST/30 | ST/45 | ST/75 | ST/150 |
|----------|-----------------|------|-------|-------|-------|-------|-------|-------|--------|
| $M = 1.3 \, M_\odot$ | [Fe/Fe] | 0.63 | 0.49 | 0.41 | 0.35 | 0.34 | 0.34 | 0.41 | 0.51 |
|          | [hs/ls] | 1.04 | 0.86 | 0.77 | 0.72 | 0.76 | 0.91 | 1.08 | 1.29 |
|          | [Pb/Fe] | 3.27 | 3.24 | 3.22 | 3.21 | 3.20 | 3.18 | 3.16 | 3.13 |
|          | [Pb/hs] | 0.41 | 0.37 | 0.36 | 0.38 | 0.42 | 0.51 | 0.58 | 0.72 |
|          | [Pb/hs] | 2.23 | 2.38 | 2.45 | 2.49 | 2.44 | 2.27 | 2.08 | 1.84 |
| $M = 1.4 \, M_\odot$ | [Fe/Fe] | 1.42 | 1.22 | 1.11 | 1.04 | 1.05 | 1.16 | 1.43 | 1.65 |
|          | [hs/ls] | 1.77 | 1.54 | 1.47 | 1.52 | 1.69 | 2.09 | 2.30 | 2.41 |
|          | [Pb/Fe] | 3.86 | 3.80 | 3.78 | 3.75 | 3.74 | 3.69 | 3.62 | 3.54 |
|          | [Pb/hs] | 0.35 | 0.33 | 0.37 | 0.48 | 0.64 | 0.93 | 0.88 | 0.76 |
|          | [Pb/hs] | 2.09 | 2.26 | 2.31 | 2.23 | 2.05 | 1.60 | 1.32 | 1.13 |
| $M = 1.5 \, M_\odot$ | [Fe/Fe] | 1.69 | 1.51 | 1.46 | 1.51 | 1.66 | 2.00 | 2.25 | 2.35 |
|          | [hs/ls] | 2.11 | 1.96 | 2.04 | 2.42 | 2.60 | 2.73 | 2.83 | 2.80 |
|          | [Pb/Fe] | 4.16 | 4.10 | 4.07 | 4.02 | 3.98 | 3.88 | 3.72 | 3.60 |
|          | [Pb/hs] | 0.42 | 0.45 | 0.59 | 0.91 | 0.95 | 0.73 | 0.59 | 0.45 |
|          | [Pb/hs] | 2.05 | 2.14 | 2.03 | 1.60 | 1.38 | 1.15 | 0.89 | 0.80 |
| $M = 2.0 \, M_\odot$ | [Fe/Fe] | 1.93 | 1.68 | 1.52 | 1.41 | 1.40 | 1.51 | 1.78 | 2.00 |
|          | [hs/ls] | 2.37 | 2.08 | 1.93 | 1.88 | 2.02 | 2.41 | 2.62 | 2.73 |
|          | [Pb/Fe] | 4.29 | 4.18 | 4.14 | 4.10 | 4.07 | 4.03 | 3.96 | 3.88 |
|          | [Pb/hs] | 0.44 | 0.41 | 0.41 | 0.48 | 0.63 | 0.90 | 0.84 | 0.74 |
|          | [Pb/hs] | 1.92 | 2.10 | 2.21 | 2.22 | 2.05 | 1.62 | 1.34 | 1.15 |

Figs C4 and C5 (Appendix C, on-line material), the three s-peak predictions in the metallicity range of $-1.6 \leq [\text{Fe/H}] \leq 0$. 

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phase. Decreasing the initial AGB mass, the poison effect is visible only for efficient $^{13}\text{C}$-pocket. For higher metallicities, this effect decreases, becoming negligible at [Fe/H] = −1 (Gallino et al. 2006).

Primary $^{22}\text{Ne}$ plays a second role at low metallicities, becoming an iron seed producer for a primary $s$-process chain, depending on the adopted $^{13}\text{C}$-pocket. Even if the neutron capture cross-section of $^{22}\text{Ne}$ is very small, not only the light elements such as $^{23}\text{Na}$ and the Mg isotopes are produced, but the neutron capture chain also extends up to $^{56}\text{Fe}$, replenishing the starting seed for the production of $s$-elements. This is shown in Fig. 14, for a low $^{13}\text{C}$-pocket (ST/12) and [Fe/H] = −2.6. Even if we set the initial abundances from $^{56}\text{Fe}$ to $^{209}\text{Bi}$ to zero, some primary iron and a consistent amount of primary $s$-elements are produced. When neutrons are largely produced by the $^{13}\text{C}(\alpha, n)^{16}\text{O}$ reaction as tests with higher $^{13}\text{C}$-pockets demonstrate (e.g. a case ST × 2), a high percentage of $s$ elements is primary (produced directly by neutron capture on $^{22}\text{Ne}$), and the $s$-element abundances are about 0.2 dex lower than the standard case. The primary $^{40}\text{O}$ and $^{12}\text{C}$ produced at low metallicities act also as neutron poison during the pocket (see on-line material, Fig. C6). We tested also the poison effect of other light elements that show minor or negligible differences.

5 Na AND Mg AS INITIAL MASS INDICATORS

As discussed in Section 4, a progressive amount of primary $^{22}\text{Ne}$ is produced in the He-intershell from the CNO cycle during the H-burning shell. The effect is a primary production of $^{23}\text{Na}$ via $^{22}\text{Ne}(n, \gamma)^{23}\text{Na}$, followed by the nucleosynthesis of Mg via $^{23}\text{Na}(n, \gamma)^{24}\text{Mg}$, $^{23}\text{Na}(\alpha, n)^{25}\text{Mg}$ and $^{23}\text{Na}(\gamma)^{26}\text{Mg}$ (Mowlavi 1999; Gallino et al. 2006). This chain involves light elements up to P, including Al and Si. In Fig. 15 (top panel), we show the [El/Fe]
Figure 13. Top panel: theoretical predictions of AGB models of \( M = 1.5 M_\odot \) for a test case with no \(^{23}\)O-pocket (case ST = 0). The line with squares stands for the ordinary case, while the line with circles corresponds to a case with the cross-section of \(^{22}\)Ne(n, \(\gamma\))\(^{23}\)Ne put to zero. Bottom panel: the same as top panel but with a ST \(^{13}\)C-pocket.

Figure 14. Theoretical predictions of AGB models of \( M = 1.5 M_\odot \) and case ST/12. The line with full squares stands for the ordinary case, while the line with empty circles corresponds to a case with the initial abundances of elements from \(^{56}\)Fe to \(^{209}\)Bi put to zero.

Figure 15. Top panel: theoretical predictions of light elements for different initial masses, \([\text{Fe/H}] = -2.6\) and a ST case. Bottom panel: theoretical predictions of the light elements in the region between Ne up to Si as a function of metallicity, for an AGB model of \( M = 1.5 M_\odot \) and ST case.

predictions in the region of the light elements, in a stellar mass range of \(1.2 \leq M/M_\odot \leq 2\), for a case ST and \([\text{Fe/H}] = -2.6\). The production of the light elements as Ne, Na, Mg and P is strongly dependent on the initial AGB mass. In particular, differences higher than 2.5 dex are observed between \( M = 1.2 \) and \( 1.5 M_\odot \). The production of primary \(^{22}\)Ne increases at lower metallicity (Fig. 15, bottom panel, for a \( M = 1.5 M_\odot \) and a case ST), due to the higher production of \(^{22}\)Ne in the H-burning ashes, thus explaining the slope predicted for \([\text{Na/Fe}], [\text{Mg/Fe}]\) and other light elements. In particular, Na (and Mg) is indicator of the mass of the AGB companion which polluted the observed CEMP-s stars (Bisterzo et al. 2006b; Bisterzo et al., in preparation).

We also remind that Na can be produced in IMS models by hot bottom burning (Sugimoto 1971; Iben 1973; Karakas & Lattanzio 2003; Ventura & D’Antona 2005), which is not included in our models.

Fig. 15 (top panel), shows a huge amount of fluorine produced in AGB stars via the chain \(^{18}\)O(\(p, \alpha\))\(^{15}\)N(\(\alpha, \gamma\))\(^{19}\)F, where protons are produced via \(^{14}\)N(n, p)\(^{14}\)C, neutrons via \(^{13}\)C(\(\alpha, n\))\(^{16}\)O reaction and \(^{18}\)O via the chain \(^{18}\)N(\(\alpha, \gamma\))\(^{19}\)F(\(\beta^-\))\(^{18}\)O (Lugaro et al. 2004, 2008; Abia et al. 2009). With the addition of proton captures in the network, the prediction of \([\text{F/Fe}]\) increased by about 2 dex. We estimate a further increase by about 0.3 dex due to the primary \(^{13}\)C from H-shell (Cristallo et al. 2009a). Further discussions and improvement about fluorine, accounting for recent experimental measurements of reaction rates involved (La Cognata et al. 2010), will be given in a forthcoming paper.

6 CONCLUSIONS

We presented theoretical results of updated AGB stellar nucleosynthesis models in a mass range \(1.3 \leq M/M_\odot \leq 3.0\) and metallicities \(-3.6 \leq [\text{Fe/H}] \leq -1\). We analysed the behaviour of the three \(s\)-process peaks and their ratios \([\text{hs/ls}]\) and \([\text{Pb/hs}]\) as the initial AGB mass and the \(^{13}\)C-pocket change. Then, we presented in detail the
abundance composition in the envelope of all the elements, from carbon to bismuth.

We find a high \([C/Fe]\) already after the first TDU episode of models at low metallicities, due to the increase with the decrease in metallicity of the primary \(^{12}\)C and to an efficient TDU. We discuss the deep impact of \(^{22}\)Ne as neutron seed and neutron poison by decreasing the metallicity. This primary \(^{22}\)Ne increases with the initial mass and as a consequence Na (and Mg) is strongly produced by decreasing the metallicity. This makes Na and Mg good indicators for the initial mass of the AGB star.

The three s-peaks are strongly dependent on the choice of the \(^{13}\)C-pocket as well as the initial mass and the metallicity. \([ls/Fe]\), \([hs/Fe]\) and \([Pb/hs]\) do not have a linear behaviour with decreasing metallicity, and, depending on the \(^{13}\)C-pocket efficiency, they can cover a large range of values. Especially \([Pb/hs]\), largely produced by decreasing the metallicity, can reach 4.5 dex. By increasing the AGB mass and then the temperature at the bottom of the TP, \([ls/Fe]\) receives an increasing contribution by the \(^{22}\)Ne(\(\alpha\), \(n\))\(^{25}\)Mg reaction. Two intrinsic s-process indexes, \([hs/ls]\) and \([Pb/hs]\), are needed in order to characterize the \(s\) distribution, independent of the dilution of the AGB material on to the companion and on the TDU efficiency. The \([hs/ls]\) ratio may give a constraint on the initial mass, and it can be an indicator of the s-process efficiency as well, while \([Pb/hs]\) gives information about the efficiency of the \(^{13}\)C-pocket only.

As well as ls, hs and Pb, we predict two peaks at Sn and Hf – W, which receive a significant contribution from the s-process. Also bismuth is synthesized in these objects via neutron capture on \(^{208}\)Pb. We remark the importance of Nb measurement in CEMP-s stars, because an extrinsic AGB has \([Zr/Fe] = [Nb/Fe]\) (e.g. CS 29497-030 by Ivan et al. 2005, see Bisterzo et al., in preparation). We refer to Bisterzo et al. (in preparation) for a comparison between our AGB models and spectroscopic observations in CEMP-s stars.

This study, together with Bisterzo et al. (in preparation) is part of a series of works, planned to provide a complete picture of the s-process nucleosynthesis in AGB stars. We are planning to extend the analysis from CEMP-s stars up to solar metallicities. We will compare AGB predictions presented here with spectroscopic observations of s-enhanced disc stars of different spectral classifications (e.g. CH and barium binary stars, intrinsic post-AGBs, extrinsic or intrinsic MS, S, C stars; for previous analysis see Busso et al. 1995, 2001; Abia et al. 2001). As last analysis, we will present an update of Galactic chemical evolution results, with AGB yields of different masses and metallicities. From the whole spectrum of these studies, we aim at better understanding of the AGB nucleosynthesis.

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