Stellar evolution, nucleosynthesis and s-process in low metallicity AGB stars

Abschlussarbeit zur Erlangung des akademischen Grades
Master of Science
vorgelegt von
Christian Ritter

Supervisor: Prof. Dr. René Reifarth
Goethe-Universität Frankfurt

Co-Supervisor: Prof. Dr. Falk Herwig
University of Victoria, Canada

Abgabedatum: 22.08.2013
Abstract

Asymptotic giant branch (AGB) stars are initially low and intermediate mass stars undergoing recurrent hydrogen and helium shell burning. During the advanced stage of stellar evolution AGB stars follow after the helium core burning ceased and are located in the AGB of the Hertzsprung-Russell Diagram. One characteristic is their ability of element synthesis, especially carbon and nitrogen, which they eject in large amounts into the interstellar medium. But AGB stars also feature a slow-neutron capture process called \( s \)-process which forms approximately 50% of all elements between Fe and Bi. The initial mass function emphasizes the importance of the synthesized ejecta of AGB stars since they are much more abundant than massive stars. Therefore, the abundance evolution of many elements in the universe is drastically affected by AGB stars. In order to understand chemical evolution in the universe their behavior must be known since their first appearance. In previous times less heavy elements were produced and available. Hence AGB stars with lower heavy element content, which means lower metallicity, must be investigated. They appear to behave substantially differently than stars of higher metallicity. Another issue is that AGB stars have mass-dependent characteristics from which follows a division into low-mass, massive and super AGB stars. Super AGB stars have the most open issues due to their large masses and initial mass boundaries that separate them from massive stars. Due to large spectroscopic surveys in the last years, many low metallicity stars have been analyzed. These findings make it necessary to complement those studies through stellar modeling. This work makes a step in this direction. The AGB star masses under investigation are \( 1M_\odot \), \( 1.65M_\odot \), \( 2M_\odot \), \( 3M_\odot \), \( 4M_\odot \), \( 5M_\odot \), \( 6M_\odot \) and \( 7M_\odot \) which include low-mass, massive and super AGB stars. Metallicities of \( Z = 6 \cdot 10^{-3} \) and \( Z = 1 \cdot 10^{-4} \) (for comparison, solar \( Z \approx 0.02 \) ) were chosen. These results are an extension of already available data, covering solar and half-solar metallicity, but without super AGB stars. Therefore physics input includes mainly well-established approaches rather than new theories. New physical approaches are included due to the low metallicity which makes the results a unique set of models. Additionally, extensive \( s \)-process network calculations lead to production factors of all included elements and isotopes. The \( s \)-process signatures of those stars were analyzed. The stellar evolution simulations presented in this work have been utilized for rate and especially sensitivity studies. One approach done was to analyze \( s \)-process branchings at \( ^{95}\text{Zr} \) and \( ^{85}\text{Kr} \) for stars at \( 3M_\odot \) with \( Z = 1 \cdot 10^{-2} \) and \( Z = 1 \cdot 10^{-3} \) respectively.
# Contents

## 1 Introduction

1.1 Stars in the low-Z Universe ........................................... 1  
1.2 Stellar evolution ..................................................... 2  
  1.2.1 Pre-AGB evolution .............................................. 2  
  1.2.2 AGB stars ..................................................... 4  
  1.2.3 Endpoints of stellar evolution ................................ 6  
1.3 AGB s-process nucleosynthesis ...................................... 7  
  1.3.1 Conditions for a neutron-capture process ..................... 7  
  1.3.2 Nuclear physics ............................................... 9  
  1.3.3 Chemical evolution of s-process elements ................... 11  
1.4 Computational approach ............................................ 13  
  1.4.1 Basic equations ............................................... 13  
  1.4.2 Numerical modeling, post-processing and 1D vs 3D ........... 15  
1.5 Aims of this thesis .................................................. 16  

## 2 Stellar modeling

2.1 Computational approach .............................................. 19  
  2.1.1 Stellar simulation with MESA ................................ 19  
  2.1.2 Extended network and yield calculation ...................... 19  
  2.1.3 Choice of general model parameter ........................... 20  
2.2 Modeling the TP-AGB phase ......................................... 21  
2.3 Mass loss ............................................................. 24  
2.4 The end of the TP-AGB phase ....................................... 26  
2.5 Hot dredge-up ........................................................ 29  
2.6 MESA revision choice and consistency check .................... 30  

## 3 Results

3.1 Stellar evolution simulations ........................................ 34  
3.2 Nucleosynthesis results ............................................ 39  
3.3 s-process at low metallicity ....................................... 43  
  3.3.1 s-process in low-Z AGB stars ................................ 43  
  3.3.2 $^{23}$Na as an s-process element in low-Z low-mass AGB stars 45  
3.4 Sensitivity study of the $^{95}$Zr branching at $Z = 0.01$ ........... 48  
3.5 Isomer implementation of the $^{85}$Kr branching at $Z = 0.001$ .... 49  

## 4 Conclusion and Outlook

53
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bibliography</td>
<td>55</td>
</tr>
<tr>
<td>A Appendix</td>
<td></td>
</tr>
<tr>
<td>A.1 Production factor tables</td>
<td>1</td>
</tr>
</tbody>
</table>

II
List of Figures

1.1 HRD of a $2\, M_\odot$ star at solar metallicity ........................................ 3
1.2 Structure of a low or massive AGB star in the interpulse phase .......... 5
1.3 Structure of a low or massive AGB star during TDUP phase ............. 5
1.4 Star classification emphasizing the AGB stage and final fate of stars different initial masses ................................................................. 6
1.5 Kippenhahn diagram of a $2\, M_\odot$ star at half-solar metallicity displaying the $s$-process site .......................................................... 8
1.6 Schematic view of the isotopic chart showing a part of the $s$-process path .. 10
1.7 Logarithmic enhancement factor of elements in the stellar ejecta of a $2\, M_\odot$ star dependent of the initial metallicity .......................... 12

2.1 Outline of the mechanism beginning with stellar evolution until post-processing 20
2.2 Schematic overview of the diffusive CBM implementation .................. 23
2.3 3D spline fit of $\eta_{\text{Bloecker}}$ dependent of mass and metallicity .......... 25
2.4 Evolution of mass loss vs. star mass for different initial masses at $Z = 1 \cdot 10^{-4}$ 26
2.5 Surface velocity of a star until the convergence issue .......................... 28
2.6 Profile of $\beta$, density, opacity and radial velocity of a $6\, M_\odot$ star with $Z = 1 \cdot 10^{-4}$ at the bottom of the CE ........................................ 28
2.7 Profile of temperature gradients, diffusion coefficients and Schwarzschild boundary at the bottom of the CE ........................................ 31
2.8 Profile of H, He mass fraction, entropy, nuclear energy generation and Schwarzschild boundary at the bottom of the CE .......................... 31
2.9 Lifetime $\tau_p$ of $^{12}\text{C}(p,\gamma)$ and diffusion timescales vs. temperature .... 32
2.10 C/O surface ratios shown for a $3\, M_\odot$ star of different MESA revisions ...... 33
2.11 Core evolution of the TP-AGB shown for a $5\, M_\odot$ star of different MESA revisions ................................................................. 33

3.1 HRD of a $1.65\, M_\odot$ born-again star ................................................. 35
3.2 HRD of different evolutionary tracks until the TP-AGB stage ............... 35
3.3 Kippenhahn diagram of the 25th TP of a $7\, M_\odot$ star with $Z = 1 \cdot 10^{-4}$ 36
3.4 Dredge-up factor dependent of star mass for different initial masses at $Z = 6 \cdot 10^{-3}$ ................................................................. 37
3.5 Initial-final mass relation dependent of initial star mass ....................... 38
3.6 Kippenhahn diagram of the core evolution of a $7\, M_\odot$ star with $Z = 6 \cdot 10^{-3}$ and $Z = 1 \cdot 10^{-4}$ ................................................................. 40
3.7 Logarithmic production factor of C and O for different metallicities ........ 42
List of Figures

3.8 Logarithmic production factor of isotopes belonging to the three $s$-process peaks. ........................................... 44
3.9 Surface evolution of [hs/Fe] vs. [ls/Fe] for different initial masses at $Z = 1 \times 10^{-4}$ 45
3.10 Surface evolution of [Pb/hs] vs. [ls/Fe] for a $2 M_{\odot}$ star at different metallicites 46
3.11 Logarithmic production factor of $^{23}$Na for different metallicites 47
3.12 Logarithmic production factor of $^{23}$Na for $Z = 1 \times 10^{-4}$ with and without neutron reaction rates ........................................... 47
3.13 $\delta$-plot of zirconium comparing simulations with SiC grain data 50
3.14 Envelope mass-fraction ratio of krypton isotopes in the envelope of $3 M_{\odot}$ stars at different $Z$ ........................................... 52
List of Tables

1.1 Parameter characterizing the evolutionary stages of a $2 \, M_{\odot}$ and $5 \, M_{\odot}$ star based on the position in the HRD ................................................. 4

2.1 Adapted parameter $f$ for the diffusive CBM mechanism for different initial masses ................................................................. 23

3.1 Final core masses of low-mass, massive and super AGB stars ................. 38

A.1 Production factors of nine stable isotopes for all star masses with $Z = 6 \cdot 10^{-3}$ 1
A.2 Production factors of nine stable isotopes for all star masses with $Z = 1 \cdot 10^{-4}$ 2
A.3 Production factors of nine stable elements for all star masses with $Z = 6 \cdot 10^{-3}$ 2
A.4 Production factors of nine stable elements for all star masses with $Z = 1 \cdot 10^{-4}$ 2
List of Tables
Chapter 1

Introduction

1.1 Stars in the low-Z Universe

During the first half of the twentieth century, it was commonly assumed that all stars had the same metal composition, as confirmed by observations (Beers & Christlieb [2005]). But in 1951, the spectroscopic results of Chamberlain & Aller [1951] indicated differences in the metal content of stars. Later, theories about nucleosynthesis in stars and their changing compositions were developed (Hoyle [1954]). Hoyle [1954] followed that the ejection of stellar nucleosynthesis products lead to a buildup of metals in the universe. Older stellar generations emerged from more metal-poor environments and therefore had a lower metal content.

In the review of Burbidge et al. [1957] the buildup of heavy elements beyond iron in stars was explained by neutron capture processes. The search for low-metallicity stars was continued in the 1970s and 1980s also in order to test theories about galaxy formation (e.g. Bond [1970]). Many low-metallicity objects were found and questions arose about the lower limits of metallicity as well as the constraints on masses at low metallicity (Beers & Christlieb [2005]). With the first results of the Preston/Shectman Survey, in the present referred to as HK survey (Beers & Christlieb [2005]), a significant amount of halo stars with $[\text{Fe}/\text{H}] \leq -3.0$ were found (Beers et al. [1985]) confirming earlier discoveries. With the large progress in detailed spectroscopic observation over the last decade including further results from the HK survey as well as new results from the Hamburg/ESO survey stars have been found with metallicity down to $[\text{Fe}/\text{H}] = -5.4$ (Beers & Christlieb [2005]). Stars at low metallicities were found to feature particular stellar abundance distributions, for example strong carbon enhancements in the Carbon-Enhanced Metal-Poor stars (CEMP, [C/Fe] > 1) (Bisterzo et al. [2011]), raising many questions about their origins.

To understand the behavior of stars including their abundance features at low metallicity one has to investigate the increase of metals over stellar generations; this change is called chemical evolution (McWilliam [1997]). Of special interest for chemical evolution are low and intermediate mass stars because they dominate in numbers and reach the asymptotic giant branch (AGB) during their evolution. The corresponding region in the Hertzsprung-Russell Diagram has a similar shape as the red giant branch but with different characteristics, for example higher luminosities. The AGB phase is reached after helium core burning ceased

\[ [X/Y] = \log_{10}(X/Y)_{\text{star}} - \log_{10}(X/Y)_{\odot} \]
and is characterized by periodic hydrogen and helium shell burning. AGB stars play a crucial role in the chemical evolution of the universe because they feature nucleosynthesis reactions as part of the slow-neutron capture process ($s$-process, Burbidge et al. [1957]). The latter is responsible for a large enrichment of heavy elements, which makes up approximately 50\% of all elements between Fe and Bi (Arlandini et al. [1999]).

Different features of AGB stars exist only at low metallicities and especially the $s$-process exhibit metallicity-dependent characteristics. To understand the processes inside low-$Z$ stars and to complement the knowledge derived from observations it is necessary to simulate stars with a smaller ratio of heavy elements, so-called lower metallicity $Z$. Here, $Z = 1 - X - Y$ holds, where $X$ and $Y$ are the hydrogen and helium mass fractions respectively. In standard spectroscopy notation the metallicity $Z$ can be estimated from Eq. 1.1 assuming that iron scales down linearly with $Z$.

\[
[\text{Fe/H}] = \log_{10}(Z/Z_\odot) - \log_{10}(H/H_\odot)
\]  

(1.1)

Since the work by Gallino et al. [1998a] large progress has been made in $s$-process modeling in low- and massive AGB stars (Beers & Christlieb [2005]). However not until lately were AGB models with metallicities down to $Z = 1 \cdot 10^{-4}$ modeled in larger numbers, providing information about production of isotopes and elements for chemical evolution (grid calculations). Simulations of AGB stars at low metallicities show features that still need to be confirmed by observations, for example the hydrogen-ingestion flash (Herwig [2005]). Also stars with the lowest metallicity observed with a $s$-process signature (i.e. at $[\text{Fe/H}] = -3.1$) cannot be explained properly by AGB models (Beers & Christlieb [2005]). But Herwig [2005] argued that the $s$-process could work down to $[\text{Fe/H}] = -5.3$.

There is currently an urgent need to improve stellar evolution and nucleosynthesis models to catch up with the progress made in spectroscopy (Herwig [2005]).

\section{1.2 Stellar evolution}

The evolution of stars is a complex and diverse topic. The following description can only highlight the most important features from birth until the final stage. Presented are low- and intermediate mass stars with the AGB phase described in most detail.

\subsection{1.2.1 Pre-AGB evolution}

In the process of star formation a cloud of interstellar matter collapses under its own weight if it overcomes the gas pressure. The Jeans instability describes the behavior of a young stellar object (Kippenhahn & Weigert [1990]). The cloud then undergoes fragmentation with each fragment collapsing faster than the cloud. Contraction and cooling of the stellar object are described by the Kelvin-Helmholtz timescale $\tau_{KH} = |E_g|/L$ where $E_g$ is the gravitational energy and $L$ the luminosity. Stars with a mass of $M = 0.08 M_\odot$ and higher start hydrogen
1.2 Stellar evolution

Figure 1.1: HRD of a $2 M_\odot$ star at solar metallicity. $L$ is the stellar luminosity and $T_{\text{eff}}$ the effective surface temperature. The stages of stellar evolution are marked in different colors. Edited figure from Herwig [2005].

Table 1.1: Parameter characterizing the evolutionary stages of a $2 M_\odot$ and $5 M_\odot$ star based on the position in the HRD. The evolution stages, roughly defined by the colored areas in Fig. 1.1, have durations of $\Delta t$.

<table>
<thead>
<tr>
<th>Evol. phase</th>
<th>$\Delta t_{2 M_\odot}$ [yr]</th>
<th>$\Delta t_{5 M_\odot}$ [yr]</th>
<th>Timescale</th>
<th>dominant burning</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pre-MS</td>
<td>-</td>
<td>-</td>
<td>$\tau_{KH}$</td>
<td>-</td>
</tr>
<tr>
<td>MS</td>
<td>$1.3 \cdot 10^9$</td>
<td>$5.6 \cdot 10^7$</td>
<td>$\tau_{nuc}$</td>
<td>H core burn</td>
</tr>
<tr>
<td>RGB</td>
<td>$5.0 \cdot 10^7$</td>
<td>$3.0 \cdot 10^6$</td>
<td>$\tau_{KH}$</td>
<td>H shell burn</td>
</tr>
<tr>
<td>HB</td>
<td>$2.0 \cdot 10^8$</td>
<td>$1.1 \cdot 10^7$</td>
<td>$\tau_{nuc}$</td>
<td>He core, H shell burn</td>
</tr>
<tr>
<td>AGB</td>
<td>$2.5 \cdot 10^6$</td>
<td>-</td>
<td>$\tau_{nuc}$</td>
<td>H shell, He shell burn</td>
</tr>
<tr>
<td>WD</td>
<td>$6.3 \cdot 10^6$</td>
<td>-</td>
<td>$\tau_{WD}$</td>
<td>-</td>
</tr>
</tbody>
</table>

burning in the center, which takes place at about $T = 10^7$ K (Kippenhahn & Weigert [1990]). Proton-proton chain reactions and the carbon-nitrogen-oxygen (CNO) cycle are dominating, dependent of stellar mass. The stable hydrogen burning phase occurs in thermal equilibrium while nuclear energy withstands the gravitational force. The phase is located on the main sequence (MS) in the Hertzsprung-Russell Diagram (HRD) and the star will remain in this long-lasting state due to the large amount of fuel. The HRD for a $2 M_\odot$ star at solar metallicity from Herwig [2005] is shown in Fig. 1.1. Table 1.1 shows corresponding times and timescales of the evolutionary stages shown in the HRD for low-mass and intermediate mass stars. Values for the $2 M_\odot$ star and $5 M_\odot$ star are also from Herwig [2005] and Kippenhahn & Weigert [1990], respectively. The burning is characterized using the nuclear timescale $\tau_{nuc} = E_{nuc}/L$ where $E_{nuc}$ is the nuclear energy reservoir, that can be released (Kippenhahn & Weigert [1990]). When the star reaches hydrogen depletion in the center, the core region
becomes stable and shrinks because of gravitation. Simultaneously, hydrogen burning starts in a thin shell around the new helium core. The envelope penetrates into the hydrogen-free core when the central burning stops and material of the core is dredged up to the surface. This is the first dredge-up. The star leaves thermal equilibrium and the MS. In contrast to the core, the envelope expands due to the shell burning and a red giant, located on the red giant branch in the HRD, is born. The core contraction happens rapidly on the Kelvin-Helmholtz timescale while the star reaches cooler surface temperatures in the HRD. For stars below \( \approx 1.8 \, M_\odot \) (Herwig [2005]) hydrogen burning proceeds under mostly non-convective conditions leading to a much higher core density, gradually increasing outwards. In such cases, core contraction leads to a fully degenerated core without any chances for cooling.

Finally, when the core temperature reaches \( 10^8 \, \text{K} \) the helium burning starts with the triple-alpha (3\( \alpha \)) reaction where three helium nuclei fuse to \( ^{12}\text{C} \) (Kippenhahn & Weigert [1990]). While a non-degenerate core can cool through expansion, degenerate cores rapidly increase in temperature making the strongly temperature-dependent reaction rate even larger. What follows for stars below \( \approx 1.8 \, M_\odot \) is a few-seconds long runaway reaction, a helium flash, with a maximum luminosity of up to that of a galaxy. In such an outburst core degeneracy is removed and stable helium burning starts on the horizontal branch in the HRD (Zero Age Horizontal Branch, ZAHB in Fig. 1.1). During He-core burning on the horizontal branch, hydrogen burns in a shell surrounding the core. A resulting carbon-oxygen core emerges in the center followed by the H-shell burning. When the helium core burning ceases the star enters the asymptotic giant branch phase (AGB phase).

### 1.2.2 AGB stars

Asymptotic giant branch stars occupy a region in the HRD with a shape similar to the red giant branch, but with a much higher radius and thus higher luminosities. The early AGB phase is characterized by He-shell burning while the core contracts. In intermediate mass stars the envelope expands and cools due to He-shell burning while the helium shell stays inactive. Then, the base of the envelope penetrates into the H-free core (Busso et al. [1999]). This is called second dredge-up. When off-center carbon burning starts, approximately during the second dredge-up, the star will evolve into a SAGB star (García-Berro & Iben [1994]). Instead of a pure carbon-oxygen core, an oxygen-neon-magnesium core arises. The initial mass needed for carbon ignition is roughly \( 8 \, M_\odot \).

Finally, when the star leaves the early AGB phase the H shell ignites again while the He shell is almost inactive (Busso et al. [1999]). In this phase giants exhibit an electron-degenerated carbon-oxygen (C/O) core or in the case of SAGB stars an oxygen-neon-magnesium (O/Ne/Mg) core with roughly between \( 0.5 \, M_\odot \) and \( 1 \, M_\odot \) (Herwig [2005]). It is surrounded by a very thin He shell (\( \approx 75 \% \, ^4\text{He}, \approx 25 \% \, ^{12}\text{C} \)) and further outwards a giant convective envelope of several hundreds of solar radii. Fig. 1.2 shows a schematic structure of a low-mass or massive AGB star during H-burning phase. Hydrogen burning through CNO cycle takes place and the He shell grows while reducing the mass of the convective envelope. The H-burning ashes consist of a large amount of \( ^{14}\text{N} \) due to the bottleneck
function of this isotope. Ring arrows in Fig. 1.2 indicate convective behavior. When the He-shell conditions reach extreme values due to a partly degenerated intershell a thin-shell instability leads to a thermonuclear runaway (Kippenhahn & Weigert [1990]). During this thermal pulse (TP), helium is burned to carbon by the 3α. The burning takes place under convective conditions in the pulse-driven convective zone (PDCZ), leaving the outer part of the former He intershell carbon enriched. Those flashes are similar to the ones known from X-ray bursts of accreting neutron stars (Herwig [2005]).

The situation after the pulse is shown in Fig. 1.3 where the intershell has reached its maximum size due to the flash. The envelope expands and cools and starts to sink into the intershell. This penetration into the intershell as (1) in Fig. 1.3 is called the third dredge-up (TDUP). Intershell material, highly enriched in carbon and helium, is mixed into the envelope where it possibly reaches the surface (see (2) in Fig. 1.3). Before, these stars were defined as oxygen-rich stars and their the carbon-to-oxygen ratio was far below one. Depending on initial mass, the carbon possibly exceeds unity and a carbon star is born. Also s-process material can reach the surface in this way. The efficiency of the TDUP increases with heavier cores, envelopes and lower metallicity (Lattanzio [1989]). After reaching some minimum in mass, H burning starts and the cycle begins again. Those periodic events, the TPs, characterize the TP-AGB phase.

AGB stars can be divided into three categories depending on initial mass with distinctive features. Low mass AGB stars with initial masses $1 \leq M/M_\odot \leq 4$, the massive AGB stars with $M/M_\odot \leq 8$ and further SAGB stars with boundaries marked by the disappearance of the second dredge-up (Herwig [2005]). The values of the mass boundaries are only roughly estimated. Fig. 1.4 from Herwig [2005] clarifies the classification.

**Low-mass AGB stars**

The TDUP is strongly mass dependent and therefore the lowest masses experience little or even no TDUP with drastic consequences as described in the next section. Stars from
approximately $1.5\, M_\odot$ to $3\, M_\odot$ are efficient s-process sites (Busso et al. [1999]). Further details about the s-process will be discussed in Sect. 1.3.

**Massive AGB stars**

Even though massive AGB stars, due to their star mass, experience effective TDUP it was found that they do not become carbon stars (Herwig [2005]). This is due to burning processes at the bottom of the convective envelope (BCE). While the temperatures at the BCE for low-mass stars are too low for proton-capture reactions, massive AGB stars experience such burning reactions. This is called hot-bottom burning (HBB). Primary $^{14}\text{N}$ is efficiently produced in the stellar envelopes and is therefore an indicator of the HBB. The temperature in the PDCZ is higher for larger core masses (Fig. 11, Cristallo et al. [2009]) and for this reason the s-process is more efficient in this convective zone.

**SAGB stars**

Stars that start carbon ignition and exhibit a sub-Chandrasekhar H-free core are called SAGB stars (Herwig [2005]). The C burning starts off-center in a partly degenerated region. SAGB stars undergo a similar evolution like massive AGB stars. As expected the HBB temperatures are higher. Ventura et al. [2013] found temperatures over $10^8$ K that feature various proton capture reactions in the envelope. Another characteristic is that due to the larger initial masses the mass loss is much stronger up to some $M_\odot^{-4}\, \text{yr}^{-1}$ (Siess [2010]).

**1.2.3 Endpoints of stellar evolution**

The final terminating stage of the AGB phase is characterized by strong mass loss, which ejects the rest of the envelope. Then a planetary nebula is born. First the star evolves in the HRD to higher temperatures and then the core starts to cool connected with a decrease in luminosity. This cooling occurs on the white dwarf (WD) cooling time scale $\tau_{WD}$ while the dwarf moves down the WD cooling track (Fig. 1.1).

Low-mass stars may experience a very late thermal pulse during their pre-WD phase as reported by Duerbeck & Benetti [1996] in Sakurai's Object. As a result H-rich material is
ingested into the He-burning convective zone. Protons are burned extremely quickly through their reaction with carbon. The timescales are too short in this reactive-convective regime and cannot be calculated with normal stellar evolution codes (Herwig et al. [2011]). Then the pre-WD leaves the cooling track and undergoes a born-again evolution. The fate of a SAGB star on the other hand will either be O/Ne/Mg WD or the star will collapse and a neutron star will be born. If and when the latter occurs is still an open issue.

1.3 AGB s-process nucleosynthesis

AGB stars play an important role in chemical evolution because of their nucleosynthesis contributions. Important contributions are the large amounts of primary carbon and nitrogen produced. Also neutron-rich isotopes roughly between $^{22}$Ne and $^{26}$Mg with primary and secondary component are synthesized. Primary means hereby the independence of metallicity, while the secondary shows a dependence. But AGB stars also feature the s-process, which is responsible for a large enrichment of heavy elements, $\approx 50\%$ of all elements between Fe and Bi (Arlandini et al. [1999]). In the following, the s-process in AGB stars is explained in more detail.

1.3.1 Conditions for a neutron-capture process

The so-called main component of the s-process takes place in the He intershell and is divided into two sources operating at different locations (Gallino et al. [1998a]). At the beginning of the TP, primary produced $^{14}$N is converted into $^{22}$Ne via $^{14}$N$(\alpha,\gamma)^{18}$F, $^{18}$F$(\beta^{+},\nu)^{18}$O and $^{18}$O$(\alpha,\gamma)^{22}$Ne. At the bottom of the PDCZ temperatures reach up to $3\cdot10^{8}$ K, enough for the reaction $^{22}$Ne$(\alpha,n)$ (Gallino et al. [1998a]). During the short time of about a year neutron densities $N_n$ between $10^{9}$ cm$^{-3}$ and $10^{11}$ cm$^{-3}$ are reached (Herwig [2005]). This neutron source was believed to be the major source of neutrons for the s-process (Iben [1975]). The $^{22}$Ne$(\alpha,n)$ reaction is strongly temperature sensitive and higher temperatures create higher neutron densities. Therefore it is not effective at low temperatures in low-mass stars, though it is important in massive AGB stars as already mentioned. Since $^{14}$N is produced during each interpulse phase it becomes available for further processing in the following pulses. During the dredge-up, protons are thought to be mixed from the envelope into the intershell. Even though the physics mechanism is still unknown this mixing is an essential part of the s-process mechanism. Due to the mixing the H/$^{12}$C ratio decreases with distance from the boundary. At the end of the dredge-up protons are captured by $^{12}$C leading to the reactions $^{12}$C$(p,\gamma)^{13}$N$(\beta^{+})^{13}$C. A thin $^{13}$C-pocket develops ($M > 7\cdot10^{-5} M_\odot$ as estimated in Herwig et al. [2003a]). Closer to the convective boundary, the H/$^{12}$C is much higher, and further protons are captured by $^{13}$C with $^{13}$C$(p,\gamma)^{14}$N. For this reason a large $^{14}$N-pocket is created directly above the $^{13}$C-pocket. When the temperature finally reaches about $10^{8}$ K the mean lifetime of $^{13}$C becomes smaller than the time between two pulses (Iliadis [2008]). The reaction $^{13}$C$(\alpha,n)$ can then produce neutrons as the major s-process neutron source (Gallino et al. [1998a]). Over thousands of years during the interpulse phase
Chapter 1 Introduction

Figure 1.5: Kippenhahn diagram of a $2 \, M_\odot$ star at half-solar metallicity in Herwig [2005] displaying the s-process site. The dotted green convective boundaries enclose the light green convective zones.

$N_n$ is approximately $10^7 \, \text{cm}^{-3}$ within the pocket (Iliadis [2008]). An overview of this scenario is given in Fig. 1.5. The neutron exposure $\tau$, the time-integrated neutron flux, is between 0.2 and 0.5 mbarn$^{-1}$ within the $^{13}$C-pocket (Herwig [2005]). In contrast, the exposure in the PDCZ with $\tau \approx 0.01 \, \text{mbarn}^{-1}$ is much smaller (Iliadis [2008]). The $^{13}$C abundance, and therefore the neutron exposure, in the pocket depend on the $^{12}$C generated in the PDCZ which is itself dependent on the boundary mixing at the bottom of the PDCZ. The s-process abundance in the $^{13}$C-pocket depends on the pocket size whereas the proton mixing through the boundary influences the pocket size.

As mentioned before, boundary mixing plays an important role in s-process nucleosynthesis. But traditionally, the Schwarzschild criterion for convective boundaries in stellar simulations strictly separate convective and radiative layers preventing boundary mixing and s-process (Herwig [2005]). Unfortunately the exact mechanism of this boundary mixing is unknown, but possible mixing candidates exist, for example gravitational waves (Denissenkov & Tout [2003]) or convective overshooting (Herwig [2000]). Rotational-induced mixing (Langer et al. [1999]) has been excluded by Herwig et al. [2003a]. Since convective overshooting is the best studied and widest spread approach it is applied in all simulations presented in this thesis and described in section 2.2.

The TDUP also brings s-process nucleosynthesis products from the intershell into the envelope. This is a necessary mechanism in order to identify the products at the stellar surface.

1.3.2 Nuclear physics

Charged particle-reactions occur efficiently until the iron peak (mass number $A \approx 56$), where the Coulomb barrier suppresses further reactions due to the maximum binding energy per nucleon in this mass region. Continuing charged-particle reactions are not energetically feasible anymore. But free neutrons, coming from s-process sources, are not affected by
1.3 AGB s-process nucleosynthesis

the Coulomb barrier. Burbidge et al. [1957] suggested that secondary iron-peak elements are seed material for the s-process from which heavier elements are synthesized due to neutron capture and β-decay. The beginning of the s-process path in the chart of nuclides is shown in Fig. 1.6. To understand the relation between neutron density and s-process path one has to look at the reaction rate per particle pair in the energy range of interest. Due to thermalization a Maxwell-Boltzmann distribution for the energy distribution of the particles can be assumed. The reaction rate per particle pair is therefore defined as Eq. 1.2.

\[
< \sigma v > = \left( \frac{8}{\pi \mu} \right)^{1/2} \left( \frac{1}{kT} \right)^{3/2} \int_0^\infty \sigma(E)E \exp \left( -\frac{E}{kT} \right) dE
\]

(1.2)

Comparing Maxwell-Boltzmann distribution with the neutron-capture cross section of \( \sigma(E) \sim 1/\sqrt{E} \) inside the integral one finds the highest product value at the maximum of the Maxwell-Boltzmann distribution. \( < \sigma v > \) is therefore dominated by this maximum. It is located at \( \approx 30 \text{ keV} \) for s-process temperatures ranging between \( 1 \cdot 10^8 \text{ K} \) and \( 6 \cdot 10^8 \text{ K} \) (Rolfs & Rodney [2005]). Finally, the reaction rate \( r \) follows in Eq. 1.3.

\[
r = \frac{N_x N_y < \sigma v >}{1 + \delta_{xy}}
\]

(1.3)

In Eq. 1.3 \( N_x \) and \( N_y \) are the number densities of particles x and y involved in the reaction. The \( \delta_{xy} \) is equal to one for identical particles and for different particles zero.

The mean lifetime of a nucleus against destruction/n-capture is described by Eq. 1.4.

\[
< \tau_{ng} > = \frac{1}{< \sigma v > N_n}
\]

(1.4)

For the low \( N_n \) in the s-process discussed above of about \( 10^8 \text{ cm}^{-3} \) results a lifetime of about ten years (Iliadis [2008]) which is much larger than the β-decay lifetimes \( \tau_\beta \) of isotopes near stability of seconds up to years (Rolfs & Rodney [2005]). Neutron-capture reactions away from the valley of (β-)-stability into neutron-rich regions are stopped by β-decays. The s-process path stays close to the valley of stability. The amount of seeds also has a large influence on the s-process distribution. An increased average number of neutrons per seed \( n_c \) (\( \approx 10 \) for main s-process, Iliadis [2008]) results in an enhanced production of heavy nuclei.

Another feature is revealed in Fig. 1.6. Following the network the last almost vertical flow is related to the neutron number 50. Due to the nuclear shell model particularly stable configurations are reached for closed shells similar to the electron shell model. These energetically favored configurations exist for neutrons with numbers 2, 8, 20, 28, 50, 84 and 126 and are called magic neutron numbers. Magic number nuclei have low neutron cross sections and therefore the s-process path cannot overcome the neutron magic number easily.

β-decays help to reach isotopes closer to the valley of stability with larger neutron-capture cross sections and the path can finally pass the magic number by neutron capture as shown in Fig. 1.6. These waiting points result in an enhancement of isotopes at magic numbers.
Figure 1.6: Schematic view of the isotopic chart showing a part of the s-process path. Starting from the iron seed the reaction path up to the first magic number \( N = 50 \) is presented. Adaption of Fig. 1 in Käppeler et al. [2011].

After the neutron flux ceases those enhancements will be in the final distribution. Therefore three s-process abundance peaks are found in the solar distribution representing the three magic numbers. In the end the s-process flux reaches \(^{209}\text{Bi}\), the most massive stable nucleus. Heavier nuclei experience \( \alpha \)-decay and for this reason the flux cannot reach further.

The s-process is divided into two components. One is the weak component which produces elements until the first s-process peak \((A = 90)\) and takes place in massive stars. The second component is the main s-process component, which produces more massive elements including the second s-process peak \((A = 140)\) until the third s-process peak \((A = 204)\). A strong component was originally thought to be responsible for the third s-process peak between \(^{206}\text{Pb}\) and \(^{209}\text{Bi}\) but it was found to originate from the main component in low-Z stars (Gallino et al. [1998a], down to \([\text{Fe/H}] = -1.6\)).

Neutron poisons and their reactions, e.g. \(^{14}\text{N}(n,p)\) have a strong influence on the s-process as they consume neutrons and change the neutron exposure. But also competing reactions like \(^{22}\text{Ne}(\alpha,\gamma)\) play an important role.

Certain unstable isotopes in the s-process path have decay times comparable to the competing neutron capture times. The s-process path split at their location and because of the split the isotopes are called branching points. The neutron source in the PDCZ plays an important role for branching points. There, high neutron densities decrease the neutron-capture lifetime. For this reason, the chance for neutron capture before decay becomes higher which alters the branching point behavior significantly. Branching points are used as indicators of temperature because higher temperatures feature higher neutron densities. Branching point ratios of meteoritic SIC grains from AGB stars allows to test the s-process conditions. Knowing the cross sections of branching point species is crucial. Therefore large effort has been made to measure s-process capture cross sections of stable, and in recent years unstable isotopes in the laboratory. Branching point nuclei have been studied in the past, for example
at DANCE (Reifarth et al. [2006]) and are the subject of further research, i.e. at the facility FRANZ in Frankfurt a. M., Germany (Reifarth et al. [2011]).

1.3.3 Chemical evolution of s-process elements

The chemical evolution started with the first stars of Population III (PopIII). Even though they are not observed yet it is thought that the first stars were massive, emerged out of big-bang nucleosynthesis material (Z = 0), and formed the first metals (Cowan & Sneden [2006]). In the following generations of PopII the iron content together with \( \alpha \)-elements increased mainly due to supernovae (SN) type 2. AGB stars contributed to the chemical enrichment relatively late due to their long lifetimes. Finally, with the onset of SN type 1a the iron production continued but without \( \alpha \)-element production resulting in a decrease of [\( \alpha/\text{Fe} \)] (McWilliam [1997]). PopI ([Fe/H] = 0) stars are metal rich stars and include our sun and the youngest stars with the highest metallicity in the Galaxy (Iliadis [2008]).

Reproducing the solar system main component is an important test of galactic chemical evolution. AGB stars experience an increase in iron content of their initial abundance during chemical evolution. This has significant implications on their s-process mechanism as seen in Fig. 1.7 from Busso et al. [1999]. There the logarithmic enhancement factor of elements dependent of initial metallicity for a 2 \( M_\odot \) star were calculated. This factor is basically the stellar yield of the element, which is the amount of mass of the element lost through winds, divided by the element’s solar abundance. The general effect seen in all panels is that at very low metallicity the yield decrease with the decreasing metallicity. The reason is that a lower amount of iron seeds are available which means less s-process elements can be produced. Also the maxima shifts from the first s-process peak (top panel) to the second s-process peak (Ba, La, Ce, Pr, Nd, Sm, middle panel, Fig. 1.7). This is because the average number of neutrons per seed \( n_c \) increases for lower metallicities and heavier nuclei can be easily reached and build up. At lowest metallicity almost all seeds are converted into nuclei of the third s-process peak, resulting in the dominance of the elements in the bottom panel. Note that even though the s-process production decreases with lower metallicity the production relative to the s-process initial abundance increases. This occurs because of the decrease in initial s-process abundances due to lower metallicity.

Studies of the neutron source \( ^{22}\text{Ne}(\alpha,n) \) reveal a clear metallicity dependence. The neutron production in the PDCZ becomes more efficient due to the increase of the temperature at the bottom for lower Z (2 \( M_\odot \) star in Fig. 11, Cristallo et al. [2009]). Branching points are activated already in low-mass stars. Intermediate mass stars were found to contribute only very little to the Galactic s-process enrichment, except in some cases, for example \( ^{96}\text{Zr} \) (Travaglio et al. [2004]).

High-resolution spectroscopic observations allow to analyze single stars at low metallicities (McWilliam et al. [1995], Beers & Christlieb [2005]). Stars enriched with s-process material like carbon stars and post-AGB stars at different metallicities were compared with model predictions and the effect of metallicity on the s-process was confirmed. Comparisons between galactic chemical evolution model results and observations were done e.g. for first
Figure 1.7: Logarithmic enhancement factor of elements in the stellar ejecta of a $2 M_\odot$ star dependent of the initial metallicity. The first till third panel includes elements of the three $s$-process peaks. Figure from Busso et al. [1999].
1.4 Computational approach

s-process elements by Travaglio et al. [2004]. Also in very metal poor environments large amounts of the third s-process peak element Pb were observed in the last decade (Beers & Christlieb [2005]). These findings confirm the current understanding.

A relation between metallicity and age is roughly found for our solar neighborhood (Garnett & Kobulnicky [2000]) but for other stellar systems, such as globular clusters, the application of this relationship may be problematic. Efforts to describe the neutron exposure dependent of metallicity have also been made with $\tau \propto 1/Z$ or $\propto Z^{-0.6}$ for different metallicity ranges (Busso et al. [1999]).

Finally, to reproduce main component of the solar system, stars of different masses and metallicity are needed as an input for a galactic chemical evolution (Lugaro et al. [2003] and references therein).

1.4 Computational approach

About a decade after the theories about star formation became more concrete in the 1950s, star formation calculations began to be seriously developed (Larson [2010]). By 1964 it was possible to simulate an intermediate-mass star until carbon burning but the lack of quantitative data for massive elements was a major constrain in calculating more advanced stages (Hofmeister et al. [1964]). Since then data from observations and nuclear experiments together with increasing computer power has allowed whole evolution sequences to be simulated, including the macro and micro physics. The basics of the common approach will be briefly introduced in the following.

1.4.1 Basic equations

Six basic differential equations describe the fundamental behavior of a star. The first three equations, Eq. 1.5a - 1.5c, are derived from conversation laws of mass, momentum and energy with the assumption of spherical symmetry (1D) and the enclosed mass in Lagrangian coordinates (Kippenhahn & Weigert [1990], Herwig [2013]).

\[
\frac{\partial r}{\partial m} = \frac{1}{4\pi r^2 \rho} \quad (1.5a)
\]

\[
\frac{\partial P}{\partial m} = -\frac{Gm}{4\pi r^4} - \frac{1}{4\pi r^2} \frac{\partial^2}{\partial t^2} \quad (1.5b)
\]

\[
\frac{\partial l}{\partial m} = \sum_i \epsilon_i \quad (1.5c)
\]

Here, $m = m(r, t)$ represents the mass in a concentric sphere dependent of radius $r$ and time $t$ (Kippenhahn & Weigert [1990]). It is used as a mass coordinate. $r$ is the radial coordinate.
Furthermore, $\rho$ is the density, $P$ the pressure and $l$ the luminosity. $\epsilon_i$ stands for energy sources and sinks, for example the nuclear energy generation $\epsilon_n$ and neutrino loss $\epsilon_\nu$.

To include the energy transport a basic equation describes the temperature gradient $\frac{\partial T}{\partial m}$. This gradient is shown in Eq. 1.6 where $\Delta = \frac{d\ln(T)}{d\ln(P)}$ depends on the type of energy transport (Kippenhahn & Weigert [1990]). For radiation and electron conduction the radiative temperature gradient with $\Delta = \Delta_{rad}$ is chosen while convection is described by the adiabatic gradient with $\Delta_{ad}$.

$$\frac{\partial T}{\partial m} = -\frac{GmT}{4\pi r^4P}\Delta \quad (1.6)$$

The fifth equation describes the composition change due to nuclear energy generation in a zone inside the star. For each species $i$ of mass $m_i$ the change in mass fraction $X_i$ over time is described by Eq. 1.7 (Kippenhahn & Weigert [1990]).

$$\frac{\partial X_i}{\partial t} = \frac{m_i}{\rho} \left( \sum_j r_{ji} - \sum_k r_{ik} \right) \quad (1.7)$$

While $r_{ji}$ describes the rates of reactions that create specie $i$, $r_{ik}$ describes reaction rates involving specie $i$’s destruction.

Mixing processes also alter abundances, as shown in Eq. 1.8 in the form of a time-dependent diffusion equation (Herwig [2013]).

$$\frac{dX_i}{dt} = \frac{\partial}{\partial m}\left(16\pi^2 r^4 \rho^2 D(m) \frac{dX_i}{dm}\right) \quad (1.8)$$

$X_i$ is the mass fraction dependent of the radius. The diffusion coefficient $D$, which depends on the mass coordinate $m$, represents different types of mixing. The convective overshooting is described by diffusion.

It needs to be emphasized that processes represented by the basic equations work on different timescales. First, the dynamical timescale $\tau_{dyn}$ describes pressure fluctuations (Eq. 1.5b), which are about 1 hr for the sun. On the other hand, the thermal timescale $\tau_{therm}$ describes for example the time to reach temperature equilibrium (Eq. 1.5c) and represents for our pre-MS sun $\tau_{KH}$ with about $1 \cdot 10^6$ yr (Herwig [2013]). Nuclear timescales work on even longer timescales which describes stable burning over billions of years (Eq. 1.7). The timescales above are presented in table 1.1 and discussed further in Kippenhahn & Weigert [1990]. The differences by many orders of magnitudes make it impossible to simulate a star in a realistic way. Therefore, simulations are calculated in step sizes which are meaningful fractions of either thermal or nuclear timescale. Each timestep corresponds to a certain model; this is the reason a timestep is often referred as a model number.
1.4 Computational approach

1.4.2 Numerical modeling, post-processing and 1D vs 3D

Using the timestep sizes mentioned above it is clear that some properties in stars are not resolved, for example mixing processes (Herwig [2013]). Nevertheless, to compute the timesteps as well as the reaction networks involved, a proper numerical approach for these differential equations must to be found. The so called Henyey method allows the basic stellar equations to be solved by dividing the star in discrete mass elements/coordinates (grid points) from the surface to the center and approximates a solution for each element of the whole mass interval (Henyey et al. [1964]). The method calculates ordinary differential equations of type Eq. 1.9a with a fully implicit Newton-Raphson solver (Herwig [2013]). An implicit numerical approach shown in Eq. 1.9b is chosen due to the stiffness of the involved problems.

\[
\frac{dy}{dt} = f(y) \quad (1.9a)
\]

\[
\frac{\Delta y}{\Delta t} = \frac{y_{k+1} - y_k}{\Delta t} = f(y_{k+1}) \quad (1.9b)
\]

\[
G(y_{k+1}, y_k) := y_{k+1} - y_k - \Delta t f(y_{k+1}) = 0 \quad (1.9c)
\]

The quantities \( y_k \) and \( y_{k+1} \) describe the current and next timestep respectively. Even though implicit methods are more computational expensive (e.g. matrix inversions) the explicit method would require timesteps that are too small. The resulting Eq. 1.9c is a root finding problem for which the Newton-Raphson root-finding method is very well applicable (Press et al. [2007]).

But solving networks comes with an issue. With small networks, such as one that includes elements up to iron, the solving of stellar structure, mixing and burning equations together (joint operator method) is computationally feasible. In contrast this is not the case for larger networks including hundreds of \( s \)-process or \( r \)-process isotopes. These would require enormous computational times. Therefore it is common to split stellar evolution calculations. In the present case evolution calculations feature a network with most energy-generating and structure-changing reactions. This includes the energy release of reactions which alter the stellar structure. Later full network calculations are done as a post-processing method based on stellar conditions like density and temperature derived from the evolution calculation. The latter works in operator split, separating mixing and nucleosynthesis (Pignatari et al. [2013]).

Perhaps the most fundamental simplification is the reduction of dimensions from 3D to 1D, assuming spherical symmetry. Unfortunately, no existing stellar evolution code can handle three dimensions since it is not computationally feasible. Therefore the basic equations presented have only a 1D form describing a star from the center to the surface in one direction using discrete mass elements. But 1D simulations, even with high spacial resolutions of typical 2000 grid points (Herwig [2005]), cannot describe important processes. For example whether dynamic motions or mixing processes like convective boundary mixing are involved. On the other hand, the physics input for 3D simulations is even more simplified than in 1D.
Chapter 1 Introduction

models because it must be computational feasible. For example, explicit compressible (3D) simulations have to obey the Courant-Friedrich-Levy condition which defines the maximum timestep size as $\Delta t = \Delta x / v_s$ where $v_s$ is sound speed and $\Delta x$ is the spatial grid size. For existing high $v_s$ only very small time steps can be calculated. Also only simple scenarios like giant envelopes are feasible and under investigation (e.g. Porter & Woodward [2000]). One promising approach is to study certain stellar scenarios over short times in detail with 3D simulations and adapt the results as an input for 1D codes. An example is the the convective overshooting mechanism introduced by Herwig [2000].

1.5 Aims of this thesis

Of special interest are AGB stars, in particular earlier generations, because they dominate in numbers and reach the asymptotic giant branch (AGB) during their evolution. Also, as discussed, AGB stars play a crucial role in the nucleosynthesis evolution of the universe. They feature the s-process, which is responsible for a large enrichment of heavy elements making up approximately 50% of all elements between Fe and Bi (Arlandini et al. [1999]). A better understanding of previous generations of AGB stars will allow to deepen the knowledge of heavy-element evolution which leads to today’s elemental abundance distribution.

The main goal of this work is to calculate the nucleosynthesis contribution of all stable elements and isotopes of low-mass, massive and super AGB stars at $Z = 6 \cdot 10^{-3}$ as well as $Z = 1 \cdot 10^{-4}$ ($[\text{Fe}/\text{H}] = -0.52, -2.3$).

Fortunately, low metallicity stars have been found in increasing number in the last ten years due to large progress in detailed spectroscopic observations for example the HK survey and the Hamburg/ESO survey (Beers & Christlieb [2005]). High resolution spectroscopy allows to observe the metal poor stars in detail (Beers & Christlieb [2005]). The possibility for detailed simulations of the behavior of those stars needs to complement observational efforts (Herwig [2005]). Simulations may help to explain particularities found in low-$Z$ stars, such as CEMP stars (Bisterzo et al. [2011]).

Massive and super AGB stars may also help to describe the different populations at low metallicities observed in globular clusters (Herwig et al. [2012]). They seem to be the best candidates to help explain a cluster self-enrichment (Ventura et al. [2013]). By calculating the nucleosynthesis contribution of stars in this mass range further investigations can be done to understand this scenario.

Many stars at low metallicity have been simulated in recent years and efforts have been made to create mass-metallicity grids of stellar yields. For example, the FRUITY database (Cristallo et al. [2011]) contains stellar yields with a dense grid between $Z = 2 \cdot 10^{-2}$ and $Z = 1 \cdot 10^{-4}$ but only with masses from $1 M_\odot$ to $3 M_\odot$. FRUITY simulations use 700 isotopes and about 1000 nuclear processes and couple the full network with their stellar evolution code (Cristallo et al. [2011]), which makes calculations computationally expensive. An exponential boundary mixing was used to allow the formation of the $^{13}$C-pocket (Cristallo et al. [2009]). Furthermore, grid calculations were performed by Karakas [2010] including metallicities with
1.5 Aims of this thesis

\[ Z = 1 \cdot 10^{-4} \text{ until } Z = 2 \cdot 10^{-2} \text{ with masses between } 1M_\odot \text{ and } 6M_\odot \text{ and using 77 species from hydrogen to sulfur (Karakas [2010]) and almost 600 reactions. A post-processing code is in use (Church & Cristallo [2009]), which can process up to 166 species (Karakas et al. [2009]). For boundary mixing Karakas [2010] introduced an artificial partial mixing zone at the deepest extent of the TDUP to create a } ^{13}\text{C-pocket. Lau et al. [2011] extended this mass range with the same stellar evolution and post-processing codes by calculating super AGB models between } 5M_\odot \text{ and } 11M_\odot \text{ at solar metallicity. An } s\text{-process network with about 500 isotopes was used. Recently, Ventura et al. [2013] performed simulations from } 1M_\odot \text{ until } 8M_\odot \text{ for } Z = 3 \cdot 10^{-4} \text{ and } Z = 1 \cdot 10^{-3}, \text{ including SAGB stars, to compare the results with cluster observations. They used a small network without boundary mixing and therefore without a } ^{13}\text{C-pocket.}

All the previous works did not include such a dense mass grid with features presented in this thesis. Additionally, previous studies did not account for a metallicity-dependence of the mass loss. The artificial boundary mixing implementation used in this thesis allows a } ^{13}\text{C-pocket to be created including the feedback of mixing (Herwig [2000]). Its behavior of the boundary mixing needs to be investigated at low } Z. \text{ The main goal of this thesis is to calculate the production of elements, including } s\text{-process elements, between } 1M_\odot \text{ and } 7M_\odot \text{ at } Z = 6 \cdot 10^{-3} \text{ and } Z = 1 \cdot 10^{-4}. \text{ To make the results more robust, the physics implemented are not based on the latest research but instead on well established and widely accepted assumptions. Therefore, rotation and magnetic fields are not considered in this work. Also, results presented here are part of an extension of Pignatari et al. [2013]. By extending Pignatari et al. [2013] to lower metallicities, an even larger mass-metallicity grid with mainly the same physics assumptions will be available. It can be applied to galactic chemical evolution simulations.}

The first part of this thesis aims is to analyze the behavior of AGB stars at low metallicities and to find approaches to model them. In the beginning, the objective was to find the latest revisions of MESA and MPPPNP which are still consistent with Pignatari et al. [2013]. Parameters to model the TP-AGB stage at low } Z \text{ with a 1D stellar evolution code were set up. In particular, a metallicity-dependent approach of the mass loss was introduced for the first time. Additionally, an issue, also known from other codes, which results in a stop of the stellar evolution code during the TP-AGB phase was investigated. Different possible approaches to solve the issue were excluded but further investigation is clearly needed. Also a phenomenon related to burning and boundary mixing during TDUP at low metallicity was analyzed. A way to suppress this behavior was found.}

The aim of the next part of this thesis is to perform grid the calculations and analyze the stellar evolution simulations and post-processing results for low-mass, massive and super AGB stars at } Z = 6 \cdot 10^{-3} \text{ as well as } Z = 1 \cdot 10^{-4}. \text{ A dense stellar evolution mass grid including } 1M_\odot, 1.65M_\odot, 2M_\odot, 3M_\odot, 4M_\odot, 5M_\odot, 6M_\odot \text{ and } 7M_\odot \text{ was calculated, using the approaches developed in the first part of this thesis. Afterwards, metallicity and mass-dependent stellar behavior were analyzed. Also, features like H-ingestion and born-again scenarios were detected. Post-processing calculations were followed by the calculation of}
Chapter 1 Introduction

production factors of elements and isotopes for all masses and metallicities. They can be provided as an input for galactic chemical evolution.

To study the effect of metallicity on the s-process is an additional aim of this thesis. Here, the influence on sensitive points within the s-process network were checked. First, the sensitivity of the branching point of zirconium was analyzed for a 3 M\(_{\odot}\) star at \(Z = 1 \cdot 10^{-2}\). The results indicate that a disagreement between grain data and simulation can probably be explained by large uncertainties of the rates of \(^{22}\text{Ne}(\alpha,\text{n})\) and , in particular, \(^{95}\text{Zr}(\text{n,\gamma})\). Finally, for the krypton branching point \(^{85}\text{Kr}\) an isomer implementation was tested for a 3 M\(_{\odot}\) star at \(Z = 1 \cdot 10^{-3}\). The strong impact on the \(^{86}\text{Kr}/^{84}\text{Kr}\) ratio at this low metallicity showed the necessity for this new approach. The results were also compared with grain data.

The following content provides the details of this work starting with methods to model AGB stars at low metallicity.
Chapter 2

Stellar modeling

2.1 Computational approach

2.1.1 Stellar simulation with MESA

Many evolution codes deal with AGB stars, for example the Garching Stellar Evolution Code (Weiss & Ferguson [2009]), the Monash stellar structure code (Karakas & Lattanzio [2007]) and the FRANEC code (Straniero et al. [1997]). Often different reaction networks are used, dependent of the isotopes of interest, with and without post-processing methods. In this work the open-source code Modules for Experiments in Stellar Astrophysics (MESA\textsuperscript{2}, Paxton et al. [2011]) of revision 3709 was used. It is a 1D code that allows the solving of coupled structure, mixing and composition equations, including a small energy-generating network, simultaneously. Features are the adaptive mesh refinement, timestep controls and an OpenMP\textsuperscript{3} parallelism support. The latter means that MESA is able to use multiple processors on a machine. The code has been used with a post-processing method. MESA features the computation of the full sequence, starting from the pre-MS until the WD stage, with exception of the TP-AGB issue explained in section 2.4. The behavior of AGB stars has been verified by comparing MESA computations with results from the EVOL stellar evolution code (Blöcker [1995], modification: Herwig [2000]) at $Z = 2 \cdot 10^{-2}$ (under revision), $Z = 1 \cdot 10^{-2}$ and at $Z = 1 \cdot 10^{-4}$. The EVOL code has been extensively tested for many years with focus on AGB stage (Blöcker [1995]). Also it was successfully compared with observations.

2.1.2 Extended network and yield calculation

The full network is calculated with the post-processing code MPPNP of the NuGrid collaboration\textsuperscript{4}. MPPNP stands for multi-zone post-processing network parallel, emphasizing the ability of the code to post-process all zones of one timestep simultaneously within the star. Its message-passing interface (MPI) parallelism allows different machines to be used for zone calculations, resulting in an enormous speed boost. The working principle is outlined in Fig.

\textsuperscript{2}http://www.mesa.sourceforge.net
\textsuperscript{3}http://openmp.org
\textsuperscript{4}Nucleosynthesis Grid project, http://www.nugridstars.org
Figure 2.1: Outline of the mechanism beginning with stellar evolution until post-processing with MPPNP.

2.1. Temperature and density profiles and diffusion coefficients for every timestep and mass zone are the input for MPPNP. These profiles are used as conditions under which nucleosynthesis calculations are performed in each zone. These calculations can be performed on many machines. Once post-processing is done in the machines (nodes) the results are sent back to the main program and are used to calculate the parameter for the next timestep (Pignatari et al. [2013]). Again, the new network information is sent to the nodes to continue with the post-processing of the next timestep and so on. A fully implicit Newton-Raphson solver (package) with sub-timestep capability is part of MPPNP. Initial abundances are needed to start a post-processing, which must be in agreement with the MESA initial abundances (Sect. 2.1.3). A physics package provides isotopes, rates and other nuclear physics needed with over five thousand isotopes and over sixty thousand rates of various compilations (Pignatari et al. [2013]). A comfortable implementation of rate changes as well as a restart capability are featured, which allows for fast and easy sensitivity studies.

2.1.3 Choice of general model parameter

Reaction network

The simulation of low-mass and massive AGB stars included a small amount of isotopes and reactions up to $^{22}$Ne, taking into account the most important energy-producing rates. These reactions and the corresponding burning phases have the strongest impact on structure and chemical composition. For super AGB stars, which ignite carbon, this network needed to be extended to include carbon-burning reactions. The reaction rates were mostly taken from the NACRE database (Angulo et al. [1999]) with some exceptions. The NACRE compilation consists of charged-particle reaction rates for stellar temperatures.
The much larger post-processing network contained the same key rates as in MESA. Rates from other compilations like JINA REACLIB\(^5\) and KADoNiS\(^6\) were also included (see Pignatari et al. [2013] for more details).

**Initial abundance**

The initial abundance calculation tool by U. Frischknecht was used to calculate the initial abundance distributions for different metallicities. To calculate the initial composition the elemental distribution of the solar composition by Grevesse & Noels [1993] plus isotopic ratios from Lodders [2003] were used. As already mentioned the onset of SN type 1a at around \([\text{Fe/H}] = -1\) strongly lowered the ratio of \(\alpha\)-elements to iron. Therefore, an \(\alpha\)-enriched initial abundance dependent of metallicity was chosen. To include the alpha enhancement, isotopes in the alpha-chain starting from \(^{12}\text{C}\) until \(^{48}\text{Ti}\) were enhanced relative to iron. All others were scaled down equally. This was done for each alpha-isotope \(X_\alpha\) through Eq. 2.1 where \(A_\alpha\) and \(B_\alpha\) were derived from fits of halo and disk star data for metallicities \(-1 \leq [\text{Fe/H}] \leq 0\) (Reddy et al. [2006]). In the case of \([\text{Fe/H}] < -1\) applies \(A_\alpha = 0\) for Eq. 2.1.

\[
\frac{X_\alpha}{\text{Fe}} = A_\alpha [\text{Fe/H}] + B_\alpha
\]  

(2.1)

**Opacities**

MESA supports radiative and electron conducting opacities. The radiative OPAL opacity tables (see Rogers et al. [1996]) include the necessary temperature range for AGB stars of \(3.75 \leq \log(T_{\text{star}[K]}) \leq 8.7\). Those opacities were calculated from the solar abundance composition of Grevesse & Noels [1993]. For the calculation OPAL opacities of type 2 were chosen due to the relevance for the increased carbon and oxygen in the atmosphere during the AGB phase. OPAL type 2 opacities were calculated using abundances enhanced of carbon and oxygen for this reason. For low temperatures between \(2.7 \leq \log(T_{\text{star}[K]}) \leq 4.5\) the tables for radiative opacities by Ferguson et al. [2005] were used. In this regime the creation of molecules and grains becomes relevant. Especially for the mass loss on the AGB where the star becomes a C-star radiative dust-driven winds become important and a good description of opacities is essential. For the overlap of \(\log(T_{\text{star}})\) between OPAL and low-temperature opacities MESA performs an interpolation (Paxton et al. [2011]). Electron conducting opacities were included by using the tables of Cassisi et al. [1998].

2.2 Modeling the TP-AGB phase

The creation of the \(^{13}\text{C}\)-pocket during the TP-AGB phase required the mixing of protons in the He-intershell layer which is done by convective boundary mixing (CBM). This mechanism, extensively described for AGB stars in Herwig [2000], was also applied during the whole evolution sequence but experienced special treatment during the AGB phase. CBM

\(^5\)Joint Institute of Nuclear Astrophysics database, https://groups.nscl.msu.edu/jina/reaclib/db/

was treated as exponential diffusive mixing as described by Eq. 1.8 where the diffusion coefficient \( D = D_{CBM} \) shows an exponential behavior. This behavior of \( D_{CBM} \) dependent of the distance into the stable region is given in Eq. 2.2 where \( D_0 \) is the diffusion coefficient and \( H_p \) the pressure scale high at the Schwarzschild boundary, and \( r \) the distance from the latter. \( f \) is a free parameter, coming from the velocity scale height, which was defined as \( f \cdot H_p \) in Freytag et al. [1996].

\[
D_{CBM} = D_0 \exp \left( \frac{-2r}{fH_p} \right) 
\]  

(2.2)

Since \( D_0 \) is not directly extractable it is approximated by the diffusion coefficient close to the boundary on the unstable side, the distance \( f_0 \cdot H_p \) away from the boundary. A scheme is shown in Fig. 2.2. The boundary mixing shuts off at a mass coordinate where the diffusion coefficient drops to \( D_{\text{limit}} \). The overshoot description features the formation of \(^{13}\text{C}\)-pocket and \(^{14}\text{N}\)-pocket which results in \( s \)-process enriched material reaching the surface. Therefore this mechanism is absolutely necessary for the \( s \)-process. Consequences for AGB stars were investigated in Herwig et al. [2000].

The aim of this thesis was, if possible, to use the same corresponding value for \( f \) as found in Pignatari et al. [2013]. Therefore \( f_0 \) is the same as the corresponding value in the latter publication. But the values of \( f \) differ for different scenarios. Up to the AGB phase a value of \( f = 0.014 \) was applied at all convective boundaries. For the bottom of the convective envelope a value of \( f = 0.126 \) was applied during TDUP while at the bottom of the pulse-driven convective zone a value of \( f = 0.008 \) was used, as used by Pignatari et al. [2013]. An exception was for the cases \( M \geq 4 M_\odot \) where CBM in the direction to the center were reduced for H-burning and non-burning convective zones down to \( f = 0.0035 \) during the whole evolution. The motivation was to reduce the mixing of protons into the stable layer when extreme temperatures at the bottom of the envelope result in HBB during TDUP in massive and super AGB stars, and the mixed protons burn as well. In order to prevent effects of the latter, such as extreme amplification of the dredge-up as discussed in Sect. 2.5, a thirty-six times smaller value of \( f \) was chosen. The HBB during TDUP is called hot dredge-up (HDUP).

But mixing modifications at low metallicity are not only done at the bottom of the convective envelope. Modifications were also done at the bottom of the PDCZ. For \( M \geq 5 M_\odot \) the mixing at the bottom of the PDCZ was reduced by choosing \( f = 0.002 \) for \( M \geq 5 M_\odot \), as it was done in the benchmark case of test calculations of a \( 5 M_\odot \) star at \( Z = 1 \cdot 10^{-4} \) in Herwig [2004]. One reason this was done was to prevent deep penetration of the PDCZ into the core. Another reason was that it decreased the efficiency of the HDUP (Herwig [2004]).

The treatment of \( f \) is summarized in Table 2.1 where \( f_{CE} \) stands for \( f \) responsible for the convective boundary mixing at the bottom of the convective envelope. \( f_{PDCZ} \) is \( f \) for mixing at the bottom of the PDCZ. \( f_{CE} \) is split up for non-burning (label 'nonburn') and HBB conditions (label 'burn'). \( f_{PDCZ} \) is only applied at the bottom boundary of the burning PDCZ (label 'burn'),
2.2 Modeling the TP-AGB phase

Figure 2.2: Schematic overview of the diffusive CBM implementation. The diffusion coefficient $D$ dependent of length $r$ continues into the stable zone. Therefore it allows mixing from the convective zone into the stable layer. The parameters are explained in Sect. 2.2.

Table 2.1: Adapted parameter $f$ for the diffusive CBM mechanism in the range of initial masses $M$. $f_{CE}$ is hereby $f$ at the bottom boundary of the convective envelope while $f_{PDCZ}$ describes it at the bottom boundary of the PDCZ. 'burn' or 'non-burn' stands for burning or no burning at the bottom of the respective convective zone.

<table>
<thead>
<tr>
<th>$M &lt; 4M_\odot$</th>
<th>$M \geq 4M_\odot$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_{CE}$</td>
<td>$f_{PDCZ}$</td>
</tr>
<tr>
<td>burn</td>
<td>nonburn</td>
</tr>
<tr>
<td>0.014</td>
<td>0.126</td>
</tr>
<tr>
<td>0.126</td>
<td>0.002*</td>
</tr>
</tbody>
</table>

* In case of $M=4M_\odot$ $f_{PDCZ}$ is still 0.008.

A better mass resolution for the AGB phase was chosen by increasing the number of mass cells in the shells. This was done with adapted mesh refinement for H, $^4\text{He}$, $^{13}\text{C}$ and $^{14}\text{N}$ aiming to better resolve the AGB $s$-process environment. Also for a better time resolution during the interpulse phase and during TP, criteria for the decrease of timestep size were introduced that were suitable for those two sites. The effect is reflected in the large amount of models spanning the AGB phase even though it is a relatively short phase compared to the whole evolution.
2.3 Mass loss

One essential stellar feature not only of the TP-AGB phase but of the whole evolution is the mass loss. It plays a particular role during RGB and AGB stages, where the mass loss dramatically increases by orders of magnitude leaving a WD as a remnant in the end. Also, mass loss has influence on the number of thermal pulses a star undergoes and hence its composition.

RGB phase

In order to model the RGB phase a classical approach used is the semi-empirical formula shown in Eq. 2.3. This formula by Reimers [1975] is based on observations and describes the mass loss in solar mass per year. It can easily be included in stellar evolution codes due to the dependency on the basic parameter mass, luminosity and radius. An additional free fitting factor $\eta_{\text{Reimers}}$ was used as well.

$$\dot{M}_{\text{Reimers}} = -4 \cdot 10^{-13} \eta_{\text{Reimers}} \frac{LM}{R^2} \left(\frac{M}{M_\odot}\right) \left(\frac{M_\odot}{\text{yr}}\right)$$  \hspace{1cm} (2.3)

Many semi-empirical formulas have been published, for example Schröder & Cuntz [2005] who created a new formula to tie the parameter to a physical description, including surface gravity and temperature. But for consistency with the already available simulation data (Pignatari et al. [2013]) and because Reimers’ formula was successfully used in many cases, it was chosen with $\eta_{\text{Reimers}} = 0.5$. The latter value was chosen because it was used in Pignatari et al. [2013].

AGB phase

As explained in Blöcker [1995] Reimers’ mass loss formula is not applicable for the AGB phase due to the fact that too high $\eta_{\text{Reimers}}$ are needed to match the observed mass loss. One reason is the dust formation which needs to be taken into account. Therefore Blöcker [1995] proposed a new description based atmospheric calculations of Mira-like stars resulting in Eq. 2.4.

$$\dot{M}_{\text{Bloecker}} = -4 \cdot 10^{-13} \eta_{\text{Bloecker}} \frac{L^{2.7}}{M^{2.1}} \dot{M}_{\text{Reimers}} \left(\frac{M}{M_\odot}\right) \left(\frac{M_\odot}{\text{yr}}\right)$$  \hspace{1cm} (2.4)

Because of the initial composition of the star the carbon to oxygen number ratio is below one (C/O $\approx 0.3$) when entering the AGB phase. This oxygen-rich phase lasts until the TDUP increases this ratio in the convective envelope above unity as explained in section 1.2. The mass loss of the oxygen star is described by an $\eta_{\text{Bloecker}}$ of 0.01. The increased mass loss of C-stars due to dust-creation and the resulting dust-driven winds are taken into account by choosing a higher $\eta_{\text{Bloecker}}$ value in Pignatari et al. [2013] for solar and half-solar metallicity stars. To model the stars for this thesis, a metallicity dependent $\eta_{\text{Bloecker}}$ was calculated. First of all, the Bloecker mass loss was fitted to the mass loss of 2 $M_\odot$ to 6 $M_\odot$ stars at $Z = 1 \cdot 10^{-4}$ from Herwig [2004], which resulted in a $\eta_{\text{Bloecker}}$ for each mass. Then the
2.3 Mass loss

Figure 2.3: 3D spline fit of $\eta_{\text{Bloecker}}$ dependent of mass and metallicity based on Herwig [2004] and Pignatari et al. [2013]. The green circles represent the chosen additional values.

$\eta_{\text{Bloecker}}$ from Pignatari et al. [2013] was taken from the $Z = 2 \cdot 10^{-2}$ and $Z = 1 \cdot 10^{-2}$ stars. The chosen values in the latter publication are based on observations, for example the amount of carbon found in the atmosphere of C-stars and in planetary nebula as well as hydrodynamic simulations (e.g. Herwig [2005], Mattsson & Höfner [2011]). For those three metallicities, plus additional $\eta_{\text{Bloecker}}$ chosen for $Z = 2 \cdot 10^{-2}$ and $Z = 1 \cdot 10^{-2}$, a 3D spline fit in the mass-metallicity plane was produced and is shown in Fig. 2.3. The additional values of masses $4 M_\odot$, $6 M_\odot$, $7 M_\odot$, $8 M_\odot$ were chosen to follow the trend of a spline fit for one metallicity and to prevent negative values at the high-mass end (green circles in Fig. 2.3).

For $Z = 1 \cdot 10^{-4}$ the resulting simulated mass loss is shown for some masses in Fig. 2.4. The stars begin their evolution with initial masses and evolve to the right by mass loss. Even though a first small increase of the mass loss is due to the RGB phase the following evolution is dominated by AGB mass loss. With the beginning shortly below the 'knee' the AGB phase is characterized by thermal pulses shown as spikes. The phase is terminated either by a sharp decrease in mass loss when the star finally leaves the AGB stage ($1 M_\odot$ star) or due to a stop of the code as described in Sect. 2.4. As expected higher initial masses show a much larger mass loss. Also there is a trend toward a higher mass loss with lower metallicity. Strong mass loss for the SAGB stars of some $M_\odot^{-4}$ yr$^{-1}$ were also found by Siess [2010]. SAGB stars show an extremely high mass loss shortly before the code stops which is probably related to the end of the TP-AGB phase as described in the next section. The described approach is a largely simplified solution and the focus was on consistency with Pignatari et al. [2013].
2.4 The end of the TP-AGB phase

In the advanced stage of the TP-AGB phase MESA experiences a situation where it is not able to solve the stellar evolution equations anymore and stops with an error. This issue is not only found in MESA but in other codes as well, for example in the Monash stellar evolution code and in the STARS code as discussed in Lau et al. [2012]. Under the conditions of a thermal pulsating shell with already low envelope mass the bottom of the envelope experiences a very low density and gas pressure. The energy cannot be carried away effectively by convection because convection is not efficient at this low density.

Such a condition is described by Lau et al. [2012] and earlier by Sweigart [1998]. The former analyzed a 8.5 $M_\odot$ model at solar metallicity. Lau et al. [2012] shows that a jump in local luminosity or opacity can lead to a radiation pressure almost represents the total pressure. Then $\beta = P_{\text{gas}}/P_{\text{total}}$ becomes very small. In their description of the base of the convective envelope, a negative gas pressure and therefore a negative $\beta$ is possible.

In this thesis, for stars of $Z = 6 \cdot 10^{-3}$ only the 1 $M_\odot$ stars left the TP-AGB. The rest continued at some point with smaller and smaller timesteps, not continuing the evolution, and were stopped by hand. In the case of the 7 $M_\odot$ a convergence issue occurred and the code stopped by itself. Lower metallicity stars of $Z = 1 \cdot 10^{-4}$ lost their envelope until a mass of 5 $M_\odot$ almost completely, with masses smaller than 0.1 $M_\odot$ left, but then ran into smaller and smaller timesteps without reaching the WD stage. The higher masses, similar to the 7 $M_\odot$ case mentioned above, stopped with a convergence issue with 1 $M_\odot$ or with smaller envelope masses left. The 1 $M_\odot$ and 1.65 $M_\odot$ reached WD stage. Generally there was a trend with higher mass resulting in more envelope left when the code stopped.
The stop of the code has implications for the post-processing. The following implications are described assuming that the evolution would have proceeded further until the envelope would have been lost. It is still an open question if this is really the case. Even though the 7 $M_\odot$ star at $Z = 6 \cdot 10^{-3}$ underwent more than twenty pulses until the code stopped there were approximately over two times more TPs possible until the envelope mass was lost. This was estimated by extrapolating the mass loss and pulse number until all envelope material was lost. In contrast the star at $Z = 1 \cdot 10^{-4}$ had already experienced clearly more than half of the pulses it could experience in total. This means at least the star with higher metallicity contributed considerable less s-process elements than he could have contributed. Fortunately, lower masses experienced roughly four fifths or more of their pulses, again estimated as above. For stars below 5 $M_\odot$ about two pulses could not be computed which did not have a strong influence on the s-process production as compared with the TP numbers. This is important because of the high s-process efficiency in low-mass AGB stars. Finally, it can be concluded that the stop of the code had the largest influence on massive and SAGB stars and in particular the 7 $M_\odot$ star at highest metallicity.

In the following the 6 $M_\odot$ with $Z = 1 \cdot 10^{-4}$ is described in more detail. The surface velocity evolution of this star before the code stopped is shown in Fig. 2.5. Clearly an oscillation with an increase above supersonic speed can be seen. The code drastically decreased the timestep size in order to try to solve the stellar equations under these conditions. Also the profiles at the bottom of the convective envelope (BCE) of the stages before the last TP (model/timestep 37000), directly after the last TP (model 40000) and shortly before the convergence issue (model 66500) are shown in Fig. 2.6. The behavior at the bottom shows the conditions described before with an extreme decrease in $\beta$. The density shows a jump for all three conditions but shortly before the convergence issue a small sharp dent occurred at the BCE. This indicated a superadiabatic zone where $\Delta > \Delta_{ad}$ with $\Delta = \frac{d\ln(T)}{d\ln(P)}$ and $\Delta_{ad} = \frac{d\ln(T)}{d\ln(P)}_{ad}$. An inefficient convection zone was found, located at the mass coordinate of the extreme peak in the velocity plot (bottom diagram). The energy could not be carried away efficiently, leading to pulsations, originating from the BCE.

Lau et al. [2012] identified the convergence issue by the negative $\beta$ and the luminosity exceeding Eddington luminosity. Even though similar results were seen, those conditions were not found. Instead the convergence issue occurred because of the extreme pulsations, which increased with radius and the code could not handle anymore.

An investigation of this effect was done for a 3 $M_\odot$ star at solar or half-solar metallicity. The iron opacity peak which Lau et al. [2012] identified as their reason for the instability in SAGB stars was removed by them to avoid the convergence problem. Similarly, an artificial reduction of the iron content for the opacity tables was successfully applied in Pignatari et al. [2013] for stars of solar metallicity to avoid the instability (e.g. high surface velocities) until almost the end of the TP-AGB. Nevertheless no simulation successfully left the TP-AGB phase and the reduction of the iron content is not a solution for the problem.

The temperature gradient was changed artificially to make the energy transport more efficient. This was done by changing $\Delta$ artificially close to the adiabatic value only when $\Delta - \Delta_{ad}$ is greater than a threshold value and only during the TP-AGB phase. The threshold
Figure 2.5: Surface velocity vs. model number (timestep) of star until the convergence issue where the code stops. The behavior shows strong oscillations far above sound speed which result in pulsations of the envelope.

Figure 2.6: Profiles of a 6 $M_\odot$ star with $Z = 1 \cdot 10^{-4}$ at the bottom boundary of the CE. From top to the bottom are shown $\beta = P_{\text{gas}}/P_{\text{total}}$, the density $\rho$, opacity $\kappa$ as well as the radial velocity $v_r$. 
value was varied in order to avoid the convergence issue. Lower velocities followed the usage of lower thresholds. Unfortunately the point of occurrence was shifted but not avoided with this implementation.

A test was conducted to find if the energy could be carried away by mass loss. Therefore the energy loss related to the mass loss ejection, currently not implemented in MESA, was compared with the total kinetic energy of the mass shells (pulsations). Comparable energies of about $10^{40}$ erg yr$^{-1}$ were found at some point in the evolution. This suggests that MESA needs a better implementation of the mass loss than the one introduced in Sect. 2.3. This could possibly solve the problem.

Other approaches, such as the inclusion of an extra turbulent pressure term, artificially viscosity or to set the velocities to zero after each timestep were not followed further after initial unsuccessful attempts. Finally, the convergence issue needs to be investigated using hydrodynamic simulations. It is not clear if this issue is encountered by real stars. If so it would affect the yields due to the dramatic mass loss related to the instability. To avoid this problem the envelope was removed artificially if the simulations stops due to the convergence issue. This approach assumes that the rest of the envelope would be lost without being altered until the WD stage. How that star behaves in reality is not known. In the case that the evolution would proceed the envelope composition of the stars simulated would not change much, aside from most massive stars, as discussed before. The envelope to the time of the code stop was added to the already lost mass to calculate production factors.

### 2.5 Hot dredge-up

In SAGB stars, especially at low Z, hydrogen burning did not stop during the dredge-up phase (Herwig [2004]). DUP combined with this burning is called hot dredge-up (HDUP) and has some strong implications on the stellar evolution (Herwig [2004]). The hot dredge up can be identified by an increase of hydrogen luminosity close to or higher than the helium luminosity. This is because protons are mixed into the stable layer of the intershell due to the convective boundary mixing during TDUP. There, they are burned under the extreme HBB temperatures occurring in the interpulse phase of SAGB stars. In this thesis only stars with masses higher than $3M_\odot$ showed HDUP of different strength. While the $7M_\odot$ models exhibited strong HDUPs over almost all TPs, lower masses showed a decrease in strength. Also, lower-Z models showed higher hydrogen luminosities, corresponding to stronger HDUP. The low-Z models show a deep dredge-up as shown in Fig. 3.4.

The following example of a $6M_\odot$ star at $Z = 1 \cdot 10^{-4}$ was chosen to present the effect of proton burning at temperatures of approximately $9.5 \cdot 10^7$ K. Figure 2.7 shows the diffusion coefficient with and without CBM. The convective layer, determined through the Schwarzschild boundary as can be seen from the adiabatic and radiative temperature gradients, is extended through CBM into the stable layer. The hydrogen burning with $^{12}$C($p$,γ) is shown in Figure 2.8 where the energy generation shows a burning just below the Schwarzschild boundary due to the CBM. The depletion of hydrogen results in a steep entropy barrier. Normally mixing
timescales are much shorter than burning timescales. But the timescale of diffusive mixing ($\tau_{\text{diff}}$) and burning ($\tau_p$) in this scenario can approach each other.

In Fig. 2.9 $\tau_p$ dependent of temperature for constant conditions of $\rho = 60 \text{ g cm}^{-3}$ and $X(^{12}\text{C}) = 0.2$ were calculated using Eq. 1.4. The conditions are roughly found at the maximum of nuclear energy generation in Fig. 2.8. For temperatures up to the peak temperature of about $0.9 \cdot 10^{8} \text{ K}$ the rate $<\sigma v>$ of the $^{12}\text{C}(p,\gamma)$ reaction were taken from the NACRE compilation. As expected the lifetime of the protons decrease for higher temperatures.

Also shown in Fig. 2.9 are $\tau_{\text{diff}}$ estimated as $\tau_{\text{diff}} \approx \Delta r^2/D$ where D is the diffusion coefficient and $\Delta r$ the distance between Schwarzschild boundary and the bottom of the convective envelope (Goriely & Siess [2004]). Both lifetimes reach similar values and can even become equal as shown in Fig. 2.9. This results in a reactive-convective regime occur on too short timescales which cannot be properly resolved by the code. The effect of feedback due to H burning, which could not be studied by Goriely & Siess [2004], resulted in extremely deep DUP reaching even into the core. To minimize this problem, a very small value for $f$ was chosen for HBB conditions during DUP in stars with $M \geq 4M_\odot$ (Sect. 2.2). For this reason the extreme DUP was suppressed in all models. Nevertheless, the reactive-convective regime needs to be studied by using 3D hydrodynamic simulations.

The current implementation of the CBM does not allow a correct identification of the DUP phase due to ongoing hydrogen burning. The result was that a large value of $f = 0.014$ during DUP was used. And a deep DUP was found that reached even after the first pulses directly into the core. To prevent this in Sect. 2.2 a value of $f = 0.0035$ was chosen.

### 2.6 MESA revision choice and consistency check

In order to use the simulations of low and intermediate stars at low metallicity as an extension of the already available data set of Pignatari et al. [2013] both data sets must be consistent with each other. Therefore the aim was to find the latest MESA revision that was consistent with rev. 3372 of Pignatari et al. [2013]. The latter is referred to as Set 1 in the following.

It needs to be emphasized that simulation results differ already slightly when the core mass is changed by only 1 %. But even when the simulation is repeated without altering any input the solver may calculate different values due to numerical errors. These errors appear as roundoff errors and truncation errors and are results of instabilities of methods (Press et al. [2007]). Often they are amplified due to the large number of calculations performed. For example, the core mass at the beginning of the TP-AGB stage which has a strong influence on the AGB evolution changes by $\approx 0.01 M_\odot$ for a $5 M_\odot$ star changed by 1 % in initial mass. When comparing different revisions this fact must be taken into account.

MESA revisions 4631, 4442, 4028, 3723, 3709 and 3635 were compared with the rev. 3372 of Set 1 by using 3 $M_\odot$ and 5 $M_\odot$ stars at $Z = 1 \cdot 10^{-2}$. While the first four revisions mentioned above show a C/O surface ratio of larger than the two latter revision who show similar behavior than Set 1. Figure 2.10 shows this difference for rev. 4631, 3709 and Set 1.
2.6 MESA revision choice and consistency check

Figure 2.7: Radiative and adiabatic temperature gradients, diffusion coefficients with ($D$) and without CBM ($D_{\text{mlt}}$). The mass coordinates are shifted and begin with the mass coordinate at the bottom of the convective envelope $M_{\text{BCE}}$. Also shown is the Schwarzschild boundary and the BCE (red and blue dashed lines).

Figure 2.8: Hydrogen and helium mass fraction including entropy profile with nuclear energy generation $\epsilon_{\text{nuc}}$. The same mass coordinate shift is done as in Fig. 2.7. Also shown is the Schwarzschild boundary and the bottom of the convective (red and blue dashed lines).
Chapter 2 Stellar modeling

Figure 2.9: Lifetime $\tau_p$ of $^{12}\text{C}(p,\gamma)$ vs. temperature. Also the diffusion timescales $\tau_{\text{diff}}$ for different diffusion coefficients $D_{\text{CBM}}$ are plotted.

The plotted revision 3709 needed an adaption in the opacity, having the same input opacity as Set 1 and was labeled "kap". Rev. 3709 is in good agreement with Set 1. Further revisions differed considerably. Comparing the hydrogen and helium free core evolution of the 5 $M_\odot$ TP-AGB evolution with and without "kap" as shown in Fig. 2.11 reveals the good agreement of the opacity adaption. The other simulations showed a difference of more than 1 % and were therefore excluded. From rev. 3372 to 3709 many changes in MESA were done, such as changes in the equation of state, ionization and solver handling. Despite this, the main difference affecting the simulations is only the treatment of the opacities. The final choice was therefore MESA rev. 3709 with the adaption of opacities.

The same treatment needed to be done for MPPNP, since the latest version agreeing with Set 1 was sought. Pignatari et al. [2013] used rev. 1876. To the time of this work, the latest available MPPNP revision was 2819. From private communication with M. Pignatari it was clear that the rate implementation changes between those two revisions are not crucial. An almost identical network was used for the simulation presented here. A full post-processing was done of the 3 $M_\odot$ and 5 $M_\odot$ comparing it with results from Pignatari et al. [2013]. The production factors at different thermal pulses as well as s-process signatures during stellar evolution were checked against results from rev. 1876. An agreement was found which lead to rev. 2819 being the choice for the post-processing calculations.
2.6 MESA revision choice and consistency check

Figure 2.10: C/O surface ratios shown for a 3 $M_\odot$ star of MESA rev. 4631, rev. 3709 and Set 1. $t_0$ is the time at the first TP, marking the beginning of the TP-AGB phase.

Figure 2.11: Core evolution of the TP-AGB shown for a 5 $M_\odot$ star of MESA rev. 4631, rev. 3709 and Set 1. 'kap' indicates the adaption of the opacities. $t_0$ is the time at the first TP, marking the beginning of the TP-AGB phase.
Chapter 3 Results

3.1 Stellar evolution simulations

A complete stellar evolution until the WD stage is seldom possible due to the convergence issue in the TP-AGB phase. But the low mass stars are good candidates for a successful calculation. In this work, not all of the low-mass AGB stars between 1 $M_\odot$ and 3 $M_\odot$ reach the WD stage in the simulations. While the 1 $M_\odot$ stars reach the WD stage the 1.65 $M_\odot$ star at higher metallicity stops in the TP-AGB phase. For the 2 $M_\odot$ stars only the $Z = 1 \cdot 10^{-4}$ star can be successfully calculated, the higher metallicity star end in the TP-AGB phase as well. Finally, all 3 $M_\odot$ stars experience convergence issues. One very late thermal pulse appeared in a 1.65 $M_\odot$ star of $Z = 1 \cdot 10^{-3}$. This born-again scenario can be seen in Fig. 3.1. Because of the reactive-convective regime investigated by Herwig et al. [2010] the evolution could not be processed with MESA. The code stopped in this phase. Finally, the 4 $M_\odot$ until 7 $M_\odot$ calculations also stopped during the TP-AGB phase. The $Z = 1 \cdot 10^{-4}$ models between 4 $M_\odot$ until 7 $M_\odot$ showed a loop in the HRD, which was caused by immediate onset of center helium burning after center hydrogen burning ceased. The HRD in Fig. 3.2 displays this behavior. It was also found by Herwig [2004] who compared the loop with Girardi et al. [1996].

The appearance of the second dredge-up is also found to be strongly metallicity dependent. The 7 $M_\odot$ star with $Z = 1 \cdot 10^{-4}$ experienced a second DUP which reached about 0.003 $M_\odot$ into the helium-free core. The protons of the envelope were burned, which is strongly reflected in the hydrogen burning luminosity while the core mass decreases. But the 7 $M_\odot$ star with higher $Z$ did not show the core penetration. The PDCZ of this star on the other hand reached into the core for the last pulses, resulting in a decrease of the hydrogen-free and helium-free core mass.

Hydrogen ingestion

The 7 $M_\odot$ SAGB stars simulated in this work showed an ingestion of hydrogen in the PDCZ during the TP-AGB phase. As seen in the Kippenhahn diagram of the 7 $M_\odot$ star with $Z = 1 \cdot 10^{-4}$ in Fig. 3.3 the convective zones of envelope and helium flash merges. As a result the ingested protons burn under extreme conditions with a luminosity even higher than the He-flash peak luminosity. The ingestion of H inside the PDCZ is discussed by Herwig et al. [2013] who also investigated a relation with the $i$-process.
3.1 Stellar evolution simulations

Figure 3.1: HRD of a $1.65 M_\odot$ star with $Z = 1 \cdot 10^{-3}$ undergoing a born-again pulse (red star).

Figure 3.2: HRD of different evolutionary tracks until the TP-AGB stage.
Chapter 3 Results

DUP efficiency

The efficiency of the dredge-up, which is an essential part of the s-process mechanism explained in Sect. 1.3, can be described by the dredge-up parameter $\lambda_{DUP}$ as in Eq. 3.1 where $\Delta M_{DUP}$ is the dredged up mass into the convective envelope.

$$\lambda_{DUP} = \frac{\Delta M_{DUP}}{\Delta M_H} \quad (3.1)$$

$\Delta M_H$ corresponds to the growth in mass of the hydrogen core during the interpulse phase. $\lambda_{DUP}$ for low-mass stars of $Z = 6 \cdot 10^{-3}$ is shown in Fig. 3.4. The $1 M_\odot$ cases showed due to their low core masses only a couple of TPs without any DUP. This is reflected in $\lambda_{DUP} = 0$. In contrast to this finding higher core masses, e.g. $1.65 M_\odot$ with $Z = 6 \cdot 10^{-3}$ showed already DUP in their advanced TPs. The massive AGB and SAGB stars had DUP at each TP. By comparing Fig. 3.4 with higher metallicity stars, here Fig. 20 in Pignatari et al. [2013], a slightly higher efficiency is found in the lower-$Z$ stars.

Core evolution

The core evolution and especially the final WD mass plays an important role from the theoretical side as well as for observations. For example WD observations help to understand the star formation history and the chemical evolution.

The final core masses of low-mass, massive and super AGB stars are shown in Tab. 3.1. The criterion for the helium core $M_{He}$ is $X_{1H} < 10^{-4}$ where $X_{1H}$ is the mass fraction of $^1$H. The helium-free core $M_{CO}$ is defined with $X_{iHe} < 10^{-4}$. The oxygen-neon-magnesium
3.1 Stellar evolution simulations

Figure 3.4: Dredge-up factor $\lambda_{\text{DUP}}$ dependent of star mass for different initial masses at $Z = 6 \cdot 10^{-3}$.

core is defined as a core where $X_O, X_{Ne}, X_{Mg}$ are larger than $X_C$ whereas the existence of a little C/O core inside the O/Ne/Mg core is ignored (see below). $M_{\text{final}}$ is the final mass of the star, meaning the star mass of the last model calculated. In contrast to this, $M_{\text{final}*}$ describes the final star mass after the star has artificially lost the rest of its envelope.

From the initial-final mass relation it is known that a higher initial mass results in a higher final mass (Marigo [2001], Fig. 8). This behavior is clearly reflected in Fig. 3.5. Here $M_{\text{final}*}$ is taken as the final mass. The metallicity dependency, far longer theoretically known than empirically confirmed, can be found as well. Also as expected, only the SAGB stars develop O/Ne/Mg cores. A metallicity dependence of the boundary can be derived from the $6 M_\odot$ stars since only the lower-$Z$ star developed a O/Ne/Mg core. Finally, no star reaches the Chandrasekhar limit of $1.4 M_\odot$ so a supernovae as the fate can be excluded.

SAGB stars, especially the $7 M_\odot$ stars, showed a significant difference in core burning. Fig. 3.6(a) and 3.6(b) show Kippenhahn diagrams of $7 M_\odot$ stars at $Z = 6 \cdot 10^{-3}$ and $Z = 1 \cdot 10^{-4}$ representing a section of the evolution in model numbers dominated by different core burning phases. Around model number 1000 a H-free cores appeared with a boundary defined by the purple solid line. The nuclear energy generation by burning is shown in different lightness of blue while the gray areas mark convective zones. H-core burning appeared under convective conditions. Roughly at model 1500 convective He-core burning started resulting in the appearance of a helium-free core with a boundary marked by the green dashed line. Finally, carbon burning started mainly off-center inside the He-free core. A thermal flash appeared under degenerate conditions at the beginning of carbon burning (Denissenkov et al. [2013]) resulting in large gray convective pockets at models of about 3500 and 2500 for Fig. 3.6(a) Fig. and 3.6(b) respectively. Off-center burning is due to the fact that neutrino loss effectively balances the gravitational energy release in the center. This is typically found in SAGB stars (García-Berro & Iben [1994], Ventura et al. [2013]). The first flash in the lower-$Z$ case started closer to the center. In the following the high-metallicity star burned downwards in further carbon flashes while the star with $Z = 1 \cdot 10^{-4}$ burned in surface...
Chapter 3 Results

Table 3.1: Final core masses of the H-free core $M_{He}$, the He-free core $M_{CO}$ and the O/Ne/Mg core $M_{ONeMg}$ of low-mass, massive and super AGB stars with initial mass $M_{ini}$ and metallicity $Z$. Additionally shown is the final star mass $M_{final}$ also with removed envelope $M_{final}^\ast$. All masses are in units of $M_\odot$.

<table>
<thead>
<tr>
<th>$M_{ini}$</th>
<th>$Z$</th>
<th>$M_{He}$</th>
<th>$M_{CO}$</th>
<th>$M_{ONeMg}$</th>
<th>$M_{final}$</th>
<th>$M_{final}^\ast$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6e-3</td>
<td>0.55</td>
<td>0.49</td>
<td>-</td>
<td>0.55</td>
<td>0.55</td>
</tr>
<tr>
<td>1e-4</td>
<td></td>
<td>0.59</td>
<td>0.55</td>
<td>-</td>
<td>0.59</td>
<td>0.59</td>
</tr>
<tr>
<td>1.65</td>
<td>6e-3</td>
<td>0.62</td>
<td>0.58</td>
<td>-</td>
<td>0.62</td>
<td>0.62</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>0.64</td>
<td>0.61</td>
<td>-</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>2</td>
<td>6e-3</td>
<td>0.62</td>
<td>0.59</td>
<td>-</td>
<td>0.65</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>0.66</td>
<td>0.64</td>
<td>-</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>3</td>
<td>6e-3</td>
<td>0.71</td>
<td>0.69</td>
<td>-</td>
<td>0.80</td>
<td>0.71</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>0.85</td>
<td>0.84</td>
<td>-</td>
<td>0.88</td>
<td>0.85</td>
</tr>
<tr>
<td>4</td>
<td>6e-3</td>
<td>0.86</td>
<td>0.85</td>
<td>-</td>
<td>1.08</td>
<td>0.86</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>0.90</td>
<td>0.9</td>
<td>-</td>
<td>0.96</td>
<td>0.90</td>
</tr>
<tr>
<td>5</td>
<td>6e-3</td>
<td>0.95</td>
<td>0.95</td>
<td>-</td>
<td>1.69</td>
<td>0.95</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>0.99</td>
<td>0.99</td>
<td>-</td>
<td>1.06</td>
<td>0.99</td>
</tr>
<tr>
<td>6</td>
<td>6e-3</td>
<td>1.05</td>
<td>1.05</td>
<td>-</td>
<td>2.27</td>
<td>1.05</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>1.13</td>
<td>1.12</td>
<td>0.99</td>
<td>1.7</td>
<td>1.13</td>
</tr>
<tr>
<td>7</td>
<td>6e-3</td>
<td>1.16</td>
<td>1.16</td>
<td>1.10</td>
<td>5.22</td>
<td>1.16</td>
</tr>
<tr>
<td></td>
<td>1e-4</td>
<td>1.27</td>
<td>1.27</td>
<td>1.26</td>
<td>2.24</td>
<td>1.27</td>
</tr>
</tbody>
</table>

Figure 3.5: Initial-final mass relation dependent of initial star mass as extracted from the MESA calculations. The curves correspond to the different metallicities as indicated.
3.2 Nucleosynthesis results

Due to the effect of convective boundary mixing the burning flame was quenched during the downward propagation until there was not enough fuel for carbon ignition left and the burning continued outwards. This effect was analyzed in Denissenkov et al. [2013] who found a WD hybrid with a large C/O core surrounded by an O/Ne zone which is itself surrounded by a C/O shell. The \( Z = 6 \cdot 10^{-3} \) star had therefore a C/O core of \( \approx 0.14 M_\odot \) with the same structure as described in Denissenkov et al. [2013]. In contrast to this the \( Z = 1 \cdot 10^{-4} \) star burned outside from the beginning. It started almost at the center resulting in a tiny fraction of a C/O core and then followed the typical structural evolution of a O/Ne/Mg WD. The final stage of the SAGB stars were not reached and therefore the collapse into a neutron star instead of a O/Ne/Mg WD cannot be excluded. Still little is known about the possibility of a collapse and nucleosynthesis implications (Herwig [2005]).

3.2 Nucleosynthesis results

Given the fact that the post-processing calculations in this work include all stable elements with 1095 isotopes and some unstable ones for the whole stellar evolution (every 20th model) a wide range of data analysis is possible.

One aim of this work is to provide results applicable for the galactic chemical evolution. Another one is to do s-process analysis with focus on metallicity dependence and is presented in the next section. In the GCE production factors of elements and isotopes play a crucial role to explain the enrichment of the ISM (Sect. 1.3.3). The way to calculate the production factor for an isotope (or element) \( i \) due to the stellar wind of an AGB star is shown in the following. The amount of the mass of the specie lost through winds until the WD remnant stage of the time \( t_{\text{remn}} \) is the stellar yield \( M_{\text{wind},i} \). Its formula is presented in Eq. 3.2 where \( \dot{M} \) is the time-dependent mass loss and \( X_{i}^{\text{surf}} \) the time-dependent surface mass fraction of the isotope or element \( i \). The yield divided by the amount of initial abundance which would be available in the total mass lost (assuming no nucleosynthesis in the star) results in the production factor \( P_{\text{wind},i} \). The mass lost is the difference of initial mass \( M_{\text{ini}} \) and mass to the time of WD remnant \( M_{\text{remn}} \). \( X_{\text{ini}} \) represents the initial mass fraction of isotope or element \( i \).

\[
M_{\text{wind},i} = \int_{0}^{t_{\text{remn}}} \dot{M} X_{i}^{\text{surf}} dt \ [M_\odot] \tag{3.2}
\]

\[
P_{\text{wind},i} = \frac{M_{\text{wind},i}}{X_{\text{ini}}(M_{\text{ini}} - M_{\text{remn}})} \tag{3.3}
\]

Production factors are available for all isotopes in ascii tables. Also elemental production factor tables are available. Both tables for \( Z = 6 \cdot 10^{-3} \) and \( Z = 1 \cdot 10^{-4} \) are available in the appendix in Table A.1, A.2, A.3, A.4 with only nine species listed due to their large number. Also plots with production factor vs. initial mass were created, which allows for comparison with the contribution of different masses and metallicities. As an example the logarithmic production factor of the light elements carbon and oxygen for different
Figure 3.6: Kippenhahn diagrams of the core evolution of a 7 $M_\odot$ stars at different $Z$. Gray lines enclose the convective zones marked as gray areas. The purple solid line and green dashed line represent H-free and He-free cores respectively. Also displayed is the nuclear energy generation with neutrino energies subtracted.
metallicities are plotted in Fig. 3.7(a) and 3.7(b). Included in the results presented here are the data from Pignatari et al. [2013]. The low mass stars around 2 M\(_\odot\) clearly show the large amount of carbon dredged up from the intershell while the higher masses experience high enough temperatures at the BCE for HBB. Thus their carbon is destroyed and much lower production factors are reached. Because the extend of HBB is metallicity dependent the carbon destruction is much more severe at lower Z. Those effects are visible in Fig. 3.7(a). Nevertheless, higher carbon enhancements in the atmosphere for lower Z stars is due to more efficient mixing and lower atmospheric carbon initially available. Oxygen is also affected by HBB and shows a similar signature. Both, carbon and oxygen experience the strongest HBB in the 6 M\(_\odot\) star at Z = 1 \cdot 10^{-4}. Ventura et al. [2013] (Fig. 2) finds for oxygen the same minimum for their Z = 3 \cdot 10^{-4} models.
Chapter 3 Results

(a) Logarithmic production factor of carbon.

(b) Production factor of oxygen.

Figure 3.7: Logarithmic production factor of carbon and oxygen for different metallicities dependent of the initial masses.
3.3 s-process at low metallicity

3.3.1 s-process in low-Z AGB stars

The slow neutron capture process plays a special role at low metallicity. This is seen clearly when looking at the logarithmic production factors of isotopes being part of different s-process peaks. Fig. 3.8(a) shows $^{88}$Sr of the first s-process peak. Since $A < 90$ most contribution of this isotope originates from the weak component of the s-process taking place in massive stars (Käppeler et al. [1989]). But the second peak is represented by $^{138}$Ba which originates, for the most part, from the main component in low-mass AGB stars as identified by Arlandini et al. [1999]. This is reflected in the logarithmic production factors of $^{138}$Ba in Fig. 3.8(b) where the stars at solar and half-solar metallicity show their maximum at $3 M_\odot$. For lower metallicity the picture changes since the maximum shifts to $4 M_\odot$. Also a higher s-process efficiency appears which is in agreement with observations as discussed e.g. by Gallino et al. [1998a] who compared their synthetic models with galactic AGB stars. For the third s-process peak Fig. 3.8(c) shows the expected metallicity-dependent effect, with higher production for lower Z. The solar and half-solar Z stars, representing the main component, contribute only marginal. The main s-process mechanism at low metallicity here in the low-mass AGB stars plays the most important role as found by Gallino et al. [1998a]. The latter estimated a contribution of the low-metallicity main component to $^{208}$Pb of 60% and the rest from the main component at half-solar metallicity, r-process and radiogenic sources. But Fig. 3.8(c) indicates a much higher contribution with a factor of $\approx 40$ between half-solar and $Z = 1 \cdot 10^{-4}$ in the $2 M_\odot$ stars.

When monitoring the neutron flux it is also interesting to look at the s-process peak elements in relation to each other. The flux goes from iron first to the first s-process peak, then the second peak and finally enhances lead (third s-process peak). To describe the relationships the ratios usually used are the parameter $[ls/Fe]$, $[hs/Fe]$, $[hs/ls]$ and $[Pb/hs]$ where ls and hs represent the mean values of elements in the first and second s-process peak respectively. Even though many definitions exist for those parameters, in this work the descriptions as in Cristallo et al. [2011] and shown in Eq. 3.4 and 3.5 are used.

$$[ls/Fe] = \frac{1}{3} ([Sr/Fe] + [Y/Fe] + [Zr/Fe]) \quad (3.4)$$

$$[hs/Fe] = \frac{1}{4} ([Ba/Fe] + [La/Fe] + [Nd/Fe] + [Sm/Fe]) \quad (3.5)$$

One motivation is spectroscopic results from which those parameters can usually be derived and compared with (e.g. Busso et al. [2001]). Since the $1 M_\odot$ and $1.65 M_\odot$ stars do not show significant s-process contributions, they are not included in the following figures.

The ratio between ls elements and Fe indicates the efficiency of the first s-process peak production. In Fig. 3.9 the $[ls/Fe]$ evolutions for different initial masses are shown. The lower masses shown feature higher values since the $^{13}$C-pocket is more efficient. Even though the
Chapter 3 Results

(a) Logarithmic production factor of $^{88}$Sr.

(b) Logarithmic production factor of $^{136}$Ba.

(c) Logarithmic production factor of $^{208}$Pb.

Figure 3.8: Logarithmic production factor of isotopes belonging to the three s-process peaks dependent of the initial masses.
3.3 s-process at low metallicity

7 M\(_\odot\) underwent the largest number of TDUP for all masses shown his s-process efficiency is so low, below 0.1, that it is barely visible. A similar behavior shows the [hs/Fe]. But one has to keep in mind that the evolution of the models stopped in the TP-AGB stage (due to the convergence issue) when comparing them with other data, such as in Fig. 5 in Cristallo et al. [2011]. At some point the ratio between ls and hs should reach an equilibrium that is characterized by its minimum. But for the ratio between Pb and hs this is not possible since Pb is at the end of the s-process path chain. Due to the fact that \(^{12}\)C in the intershell is primary while iron seeds scale down with metallicity the neutron exposure (and s-process efficiency) in the \(^{13}\)C-pocket increases for lower Z. A higher exposure drives the neutron flux strongly up to lead. Fig 3.10 shows the evolution of the [Pb/hs] and since the ratio could grow without reaching equilibrium a clear dependency of metallicity can be seen. Solar and half-solar metallicity stars show a negative trend, indicating that the neutron flux does reach to hs but not up to lead. But for the two lowest metallicities the increase of [Pb/hs] is dramatic, already after the first pulses. The maximum [Pb/hs] of \(\approx 0.9\) for the \(Z = 1 \cdot 10^{-4}\) star is similar to the result from Lugaro et al. [2012] (Fig. 8) who investigated stars at \(Z = 1 \cdot 10^{-4}\). Also Cristallo et al. [2009] investigated the 2 M\(_\odot\) stars for different metallicities but their [Pb/hs] trend showed higher final surface ratios of up to 2.88 for \(Z = 1 \cdot 10^{-4}\). The star of lowest metallicity shows some sort of saturation which is followed by a decrease. This effect, which can also be seen in Lugaro et al. [2012] (Fig. 8), indicates a decrease in neutron exposure close to the end of the TP-AGB evolution.

3.3.2 \(^{23}\)Na as an s-proces element in low-Z low-mass AGB stars

It is widely accepted that \(^{23}\)Na is not an s-process isotope. Instead it plays an important role during HBB in massive and super AGB stars. There it is produced by proton capture at the bottom of the CE. For observers Na has spectroscopic relevance in the globular
cluster surveys. Massive and super AGB stars are suggested candidates for the enrichment of the interstellar medium in those clusters and are their $^{23}$Na production is therefore under investigation.

But the effect of metallicity on $^{23}$Na production in AGB stars was not fully taken into account as presented in the following. As can be seen in Fig. 3.11 the $^{23}$Na production strongly increased for lower metallicity in low mass AGB stars with a peak at the $2 M_\odot$. The reason was the increase of the core mass for lower $Z$ which makes HBB more efficient. But the production channel is not only dominated by proton capture during HBB on $^{22}$Ne as assumed but instead by neutron capture at $Z = 1 \cdot 10^{-4}$. This was found by comparing two post-processing networks, one including neutron reactions and one without any reactions. The results in Fig. 3.12 indicate that indeed $^{23}$Na is produced by neutron capturing during the $s$-process by over 80 %. Hence, $^{23}$Na production by AGB stars in low metallicity environments in globular cluster may be dominated by their low-mass types.

Ventura et al. [2013] investigate elements in AGB simulations of the range $1 M_\odot$ until $8 M_\odot$ of interest for spectroscopic surveys of globular clusters. They try to understand the oxygen-sodium anticorrelation observed in galactic globular clusters but find a correlation instead. They argue that at such high temperatures where a destruction of oxygen at the bottom of the envelope occurs also $^{23}$Na is destroyed by proton capture. But they do not include the $s$-process mechanism in their work and so their models do not reflect a realistic behavior. Further investigations should be done with $s$-process inclusion.
3.3 s-process at low metallicity

Figure 3.11: Logarithmic production factor of $^{23}$Na for different metallicites.

Figure 3.12: Logarithmic production factor of $^{23}$Na for $Z = 1 \cdot 10^{-4}$ with and without neutron reaction rates.
Chapter 3 Results

3.4 Sensitivity study of the $^{95}$Zr branching at $Z = 0.01$

Zirconium, discussed before as an element in the first $s$-process peak, also plays an important role for branching point studies. Due to the fact, that $^{90}$Zr, $^{91}$Zr, $^{92}$Zr and $^{94}$Zr are stable isotopes with low neutron-capture cross sections and $^{93}$Zr is a long-lived unstable isotope with low cross sections as well, the following short-lived unstable $^{95}$Zr (62 days) results in a branching point isotope. The neutron densities reached in the $^{13}$C-pocket are not high enough to create $^{96}$Zr and therefore it was traditionally an $r$-process isotope (K"appeler et al. [1989]). Later, $^{96}$Zr was identified as a $s$-process isotope for higher neutron densities, such as those higher than $\approx 4 \cdot 10^8$ cm$^{-3}$ as found in Arlandini et al. [1999]. These conditions can be reached with the help of the temperature-sensitive $^{22}$Ne($\alpha,n$) reaction in the PDCZ. Higher temperatures in the PDCZ, a feature of a higher star masses, increase the efficiency of the neutron production and therefore the $^{96}$Zr enhancement. The $^{94}$Zr on the other hand is produced in the $^{13}$C-pocket. Nevertheless, the $^{96}$Zr/$^{94}$Zr ratio is an ideal diagnostic tool for the PDCZ temperature (Herwig [2005]).

Also zirconium can be measured with the resonance ionization mass spectroscopy in SiC main-stream grains that originate in AGB stars (Gallino et al. [1990]). Gallino et al. [1998b] confirmed a multiplicity of AGB stars as a source of SiC grains by comparing solar-metallicity low-mass stars. Therefore not only one mass and metallicity can explain the distribution found in grains. Lugano et al. [2003] compared the grain data with solar-Z low-mass and massive AGB stars and found Zirconium to come from low-mass AGB stars at solar or near-solar metallicities.

A comparison of $\delta (^{90}$Zr/$^{94}$Zr) versus $\delta (^{96}$Zr/$^{94}$Zr) of a standard $3 M_\odot$ model with $Z = 1 \cdot 10^{-2}$ (label 'st') with grain data is shown in Fig. 3.13. The $\delta$-notation is typically used to present grain data. For isotope $X$ and $Y$ follows in $\delta$-notation the Eq. 3.6 where $N_X$ and $N_Y$ represents the number fraction of the corresponding isotope.

$$\delta(X/Y) = 10^3 \left( \frac{N_X}{N_Y} \left( \frac{N_Y}{N_X} \right)_\odot - 1 \right)$$  \hspace{1cm} (3.6)

From Fig. 3.13 it can be clearly seen that the models produced too much $^{96}$Zr. This outcome can be due to different reasons.

Unfortunately, due to the half-life of 62 days of $^{95}$Zr, its neutron capture cross section has not been measured yet and nucleosynthesis codes must rely on theoretical models. As can be seen from KADoNIS the theoretical rates vary within a range of 24.2 mb until 139.7 mb at a energy of 30 keV, while the value taken in this work is 79 mb. It was therefore necessary to investigate the rate change of $^{95}$Zr($n,\gamma$).

Another issue is the important rate of $^{22}$Ne($\alpha,n$) which is still uncertain by some factors. In this work the experimental (recommended) rate of $N_\alpha < \sigma v >= 1.6 \cdot 10^{-13}$ cm$^3$ mol$^{-1}$ s$^{-1}$ at 2.5 $\cdot$ 10$^8$ K by Jaeger et al. [2001] was used. The latter used higher resolution and an additional resonance for the rate calculation compared to previous work (NACRE, K"appeler
et al. [1994]). While the rate uncertainty by NACRE was about 500, Jaeger et al. [2001] could reduce the uncertainty to be a factor of 100. The most recent results are from Longland et al. [2012] who used new experimental data and a Monte-Carlo method to estimate the neutron source reaction rate. A recommended rate of \( N_A < \sigma v > = 2.06 \cdot 10^{-13} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \) at 2.5 \( \times \) 10\(^8\) \text{ K} for the neutron source was found and their lower limit is still above the recommended rate of Jaeger et al. [2001]. In a direct comparison of the uncertainty bands of Longland et al. [2012] with Jaeger et al. [2001], Fig. 4, shows a narrower band and with that the improvement of the rate uncertainty. From the reaction rate probability density function they derived for 68 % and 95 % rates which are smaller than a factor two of their recommended value for 2 \( \times \) 10\(^8\) \text{ K}.

Also it needs to be mentioned that the CBM description used in this work has a strong impact on the temperature at the bottom of the PDCZ and therefore on the rate efficiency of \(^{22}\text{Ne}(\alpha,\text{n})\) (Herwig [2000]). But since the value of \( f \) is finely tuned (Sect. 2.2) a change of the parameter was not considered.

Therefore, to test the influence of the \(^{22}\text{Ne}(\alpha,\text{n})\) rate as well as the \(^{95}\text{Zr}(\text{n,}\gamma)\) additional calculations for a 3 \( M_\odot \) star at \( Z = 1 \cdot 10^{-2} \) were performed. First, the \(^{22}\text{Ne}(\alpha,\text{n})\) rate was decreased by a factor of 2 to take roughly into account the uncertainty of the rate and shown in Fig. 3.13. But since the latest rate uncertainties are above this value and the minor shift in the diagram more priority must be set on the \(^{95}\text{Zr}(\text{n,}\gamma)\) rate. This rate was decreased by a factor of two as well and finally both rates were decreased together by a factor of two. The results show a clearly better similarity between SiC grain data and simulation. The grain data is taken from Mainstream grains which possibly origin from the envelope of AGB stars. The run with changes of both rates was found to be the best candidate. Due to the fact that the \(^{95}\text{Zr}(\text{n,}\gamma)\) still has a large uncertainty, a test with a decrease by a factor of four should be done too. As emphasized by Lugaro et al. [2003] the stars below 3 \( M_\odot \) are also important contributor to the \(^{96}\text{Zr}/^{94}\text{Zr}\) ratio. Even though the results look promising, this topic needs further investigation. For example, through making further rate changes and by using lower initial masses.

### 3.5 Isomer implementation of the \(^{85}\text{Kr}\) branching at \( Z = 0.001 \)

Unlike zirconium, krypton is a noble gas but also includes a s-process branching point. It is located at the unstable \(^{85}\text{Kr}\). The isotope is surrounded by stable pure s-process nuclide \(^{84}\text{Kr}\) and the neutron magic isotope \(^{86}\text{Kr}\). The particularity of the branching point arise from an isomeric state \(^{85m}\text{Kr}\) which is occupied by \( \approx 50 \% \) when capturing a neutron. While \(^{85}\text{Kr}\) (ground state) features a half-life of 10.76 years \(^{85m}\text{Kr}\) comes with a much shorter half-life of 4.48 hours. To draw conclusions from the \(^{85}\text{Kr}/^{84}\text{Kr}\) ratio of stellar simulations it is therefore necessary to include the isomeric state \(^{85m}\text{Kr}\) into network calculations. In the past, isomers have often not been included into the reaction network. In calculations presented so far, only isomers of \(^{26}\text{Al},^{85}\text{Kr},^{115}\text{Cd},^{176}\text{Lu}\) and \(^{180}\text{Ta}\) are taken into account. They
Figure 3.13: $\delta$-plot of zirconium comparing simulations of a $3\ M_\odot$ star at $Z = 1 \cdot 10^{-2}$ with grain data from SiC grains. Shown are the standard simulation, simulations with reduction of the $^{22}\text{Ne}(\alpha,\text{n})$ rate and $^{95}\text{Zr}(\text{n},\gamma)$ rate by a factor of two and a calculation with the change of both rates by a factor of two ('Mix').

are treated as a separate species if the conditions are below a thermalization temperature ($^{85}\text{Kr}: T_\text{therm} = 5 \cdot 10^8$ K) and then terrestrial rates are used (see Pignatari et al. [2013]). 42 % of the production of $^{85}\text{Kr}$ goes into the isomeric state. The difference to 50 % is due to the decay of $^{85m}\text{Kr}$ into its ground state and the decay is therefore treated independently of temperature. Obviously this implementation is not realistic and a preliminary approach was done by Thomas [2013] who included the isomer $^{85m}\text{Kr}$ at solar metallicity as a separate particle, dividing $^{85}\text{Kr}$ into a possible ground and isomer state. Rates were calculated in a more realistic energy-dependent way for both states using the level data and $\gamma$-transitions from NNDC\(^7\).

In order to estimate the effect of the new isomeric state implementation at low $Z$ two $3\ M_\odot$ stars at $Z = 1 \cdot 10^{-3}$ were simulated, with ('isomer') and without ('standard') new implementation. The influence on the krypton isotope abundances of both cases are shown in Fig. 3.14. There, the mass-fraction ratios of krypton isotopes, $^1\text{Kr}$ divided by $^{82}\text{Kr}$, in the envelope dependent of the mass number $A$ are plotted. They are normalized to solar values of Lodders [2003] which means that all stars simulated begin their evolution with the solar ratio of 1 (horizontal line in Fig. 3.14). The reason was that in order to obtain the initial abundances for $Z = 1 \cdot 10^{-3}$ the solar abundance distribution was scaled down without changing krypton ratios (Sect. 2.1.3). The data of isomer and standard implementation is taken from the end of the TP-AGB phase where the isomer implementation altered the envelope the most. As expected the new approach did not influence other krypton isotopes except $^{86}\text{Kr}$. Fig. 3.14 reveals almost a factor of 1.8 in production of $^{86}\text{Kr}$. This shows that

\(^7\)http://www.nndc.bnl.gov/
the new isomeric implementation urgently need to be included into simulations in order to allow accurate comparisons with observations. The results from the standard simulation were confirmed by the comparison with simulation data of a 3 $M_\odot$ star at $Z = 1 \cdot 10^{-3}$ from the FRUITY database (except for $^{78}$Kr where no data was available). From the latter the mass fraction ratios after the last TDUP episode were taken. Also their initial abundances is derived by scaling down of Lodders [2003]. The standard and FRUITY data are in good agreement as shown in Fig. 3.14. One reason may be that the FRUITY database uses a similar approach as in the standard case with the same ratio between the reaction into the ground and isomeric state (Straniero et al. [2006]).

Krypton can be measured in grains. The grains originate in AGB envelopes of carbon stars from where the simulation data of Fig. 3.14 was also taken. Therefore the figure can be compared with grain data of Fig. 1 in Pignatari et al. [2006]. The data of the latter were taken from Lewis et al. [1994], who analyzed 5 noble gases including Krypton from the Murchison meteorite. The high $^{86}$Kr/$^{82}$Kr ratios plotted in Pignatari et al. [2006] cannot be reached with standard isomer implementation of a $3 \ M_\odot$ star at $Z = 2 \cdot 10^{-2}$ (Thomas [2013]). Thomas [2013] reached a better agreement for higher $^{86}$Kr/$^{82}$Kr grain ratios by using the isomer implementation for the same star. Still, roughly a factor of two is needed to reach the highest grain ratio. This maximum in the grain data agrees with the maximum of $^{86}$Kr/$^{82}$Kr in the standard simulation at $Z = 1 \cdot 10^{-3}$ plotted in Fig. 3.14. It is also within the range between initial and the maximum grain ratio of the new implementation and can therefore also be explained with it. The neutron capture cross section of $^{85}$Kr is only a theoretical value with large uncertainties (Pignatari et al. [2006]) which is a motivation for radioactive isotope measurements.

Grains originate from AGB stars of different metallicities and masses (Lewis et al. [1994]). This confirms the findings described before. But Pignatari et al. [2004] excluded stars below $Z = 6 \cdot 10^{-3}$ to be responsible for the $^{86}$Kr/$^{82}$Kr spread of grain data in Fig. 1 in Pignatari et al. [2006] by comparing the $^{134}$Xe/$^{130}$Xe ratios in different simulations down to $Z = 3 \cdot 10^{-3}$ with the grain data.

Additionally, a comparison of grain data with simulations of this work is not possible due to the age of the grains. From interstellar residence lifetime measurements Heck et al. [2009] found a lifetime of up to $1.1 \cdot 10^9$ yr based on $^{21}$Ne and $^3$He produced by Galactic cosmic rays. From a revised age vs. metallicity relation of the solar neighborhood presented in Fig. 1 of Garnett & Kobulnicky [2000] it can clearly be seen that $10^9$ yr corresponds to a metallicity far above [Fe/H] = $-1.3 \ (Z = 1 \cdot 10^{-3})$. Therefore the performed simulations down to the [Fe/H] = $-2.3$ cannot be compared directly with grain data. Including the stellar lifetime of $\approx 3 \cdot 10^8$ years of the $3 \ M_\odot$ star does not change this result.

Nevertheless Lewis et al. [1994] extrapolated the $^{86}$Kr/$^{82}$Kr ratio in grains to smaller $^{84}$Kr to $^{82}$Kr ratio. The latter decreases with decreasing metallicity (Gallino et al. [1990]). They found an increasing spread for lower $Z$ due to the different grain sizes which can be confirmed in Fig. 3.14. By comparing $^{86}$Kr/$^{82}$Kr of $Z = 1 \cdot 10^{-3}$ with solar metallicity $Z = 2 \cdot 10^{-2}$ (Pignatari et al. [2013]) one find a clear dependence of the $^{86}$Kr/$^{82}$Kr ratio with metallicity in simulations, with lower metallicity featuring a higher value. The large ratio at the end...
Figure 3.14: Envelope mass-fraction ratios of krypton isotopes $^{41}\text{Kr}$ divided by $^{82}\text{Kr}$ of $3 \, M_\odot$ stars dependent of the mass number $A$ at the end of the TP-AGB phase. FRUITY data is taken after the last TDUP episode. The ratios are normalized to solar values. Compared is the standard implementation with results of the isomer implementation ('isomer') and the data from the FRUITY database at $Z = 1 \cdot 10^{-3}$. Additionally, krypton isotopes at solar metallicity from Pignatari et al. [2013] are plotted.

of the TP-AGB phase could explain even the largest $^{86}\text{Kr}/^{82}\text{Kr}$ in Lewis et al. [1994] when taking into account the new isomer implementation. All ratios of the star at solar metallicity are below 1. The reason for this is that the krypton isotope ratios in the solar composition, which exist initially in the envelope, are produced by the $s$-process and $r$-process. Then, the pure $s$-process material dredged-up into the envelope lowers the ratio of isotopes shown in Fig. 3.14 to which the $r$-process contributed.
Chapter 4

Conclusion and Outlook

Stellar evolution and nucleosynthesis in AGB stars at low metallicity are far from being completely understood.

Therefore it is the challenge of this work to model AGB stars at $Z = 6 \cdot 10^{-3}$, $Z = 1 \cdot 10^{-3}$ and $Z = 1 \cdot 10^{-4}$ covering low-mass, massive and super AGB stars. A fine mass grid with masses of $1 M_\odot$, $1.65 M_\odot$, $2 M_\odot$, $3 M_\odot$, $4 M_\odot$, $5 M_\odot$, $6 M_\odot$ and $7 M_\odot$ were included. Hereby new approaches for calculations at low metallicity were developed and findings were investigated. Worth mentioning is the new mass- and metallicity-dependent mass loss. Low-metallicity phenomenon like the HDUP or H-ingestion during the TP were found. Additionally the $s$-process nucleosynthesis were analyzed and production factors of elements and isotopes calculated. Finally, $s$-process branching points were studied. The first branching studied was the $^{95}$Zr branching. The disagreement between grain data and simulation of a $3 M_\odot$ star at $Z = 1 \cdot 10^{-2}$ at this branching point can probably be explained by large uncertainties of the rates of $^{22}$Ne$(\alpha,n)$ and especially $^{95}$Zr(n,$\gamma$). The trend shows a better agreement with grain data which reveals the need for rate measurements of radioactive isotopes. With the ability to measure radioactive isotopes with a half-life of tens of days the FRANZ facility in Frankfurt a. M., Germany, may be able to measure the extremely uncertain $^{95}$Zr(n,$\gamma$) cross-section (Reifarth et al. [2011]). Also the $^{85}$Kr branching was investigated. A new isomer implementation for $^{85}$Kr was tested using a $3 M_\odot$ star at $Z = 1 \cdot 10^{-3}$. The results show the strong impact and, consequentially, the necessity of a correct treatment of the $^{85}$Kr isomer.

To continue the study, the next steps would be the following:

- The verification process can be followed by further validation which includes a comparison with other simulations and observations.

- To complete the extension of models of Pignatari et al. [2013] it will be necessary to add another metallicity at $Z = 1 \cdot 10^{-3}$. This will allow to provision of a unique dense mass and metallicity grid of models for many applications.

Also the issues and features found during this work offer great possibilities for continuing the investigation in different directions. Future topics might further consider those findings that clearly showed the limits of current simulations.
One issue is related to the handling of the end of the TP-AGB phase. Even though it is a widely known issue that stellar evolution codes do not converge not much progress was achieved in the past. It is worth putting efforts into this topic to understand mass loss and PN formation.

Another problem is related to the $s$-process. The size of the $^{13}$C-pocket cannot be reproduced in the correct size with the current overshooting implementation. The size is about 3 times smaller than the estimates of $M > 7 \cdot 10^{-5} M_\odot$ by Herwig et al. [2003b]. A new approach currently under investigation and based on gravitational waves, extend the overshoot description at convective boundaries (Battino [2013]). This may help to produce large enough pockets and may be incorporated in future simulations.

The HDUP needs to be investigated in more detail. The treatment of the overshooting as shown in this work is only a temporary solution. One approach may be to use 3D hydrodynamic simulations to approach the problem of burning and mixing.

Generally, the main obstacle is to understand the (nonstandard) mixing processes involved in AGB evolution because of their enormous importance. 3D hydrodynamic simulations may therefore be the best way to go. Steps in the direction of reactive mixing should be done to investigate possible feedback.

Nevertheless, 1D simulation and nucleosynthesis tools, which allow full stellar sequences to be processed, are great tools. With the complexity of macro and micro physics included in these tools, they open the way to connect different research areas. Starting from meteorite studies over stellar spectroscopy to chemical evolution of galaxies, many research fields are included and more may be in the future.
Bibliography


Battino, U. 2013, personal communication 4

Beers, T. C. & Christlieb, N. 2005, Annual Review of Astronomy and Astrophysics, 43, 531 1.1, 1.1, 1.3.3, 1.5

Beers, T. C., Preston, G. W., & Shectman, S. A. 1985, AJ, 90, 2089 1.1

Bisterzo, S., Gallino, R., Straniero, O., Cristallo, S., & Käppeler, F. 2011, ArXiv e-prints 1.1, 1.5


Burbidge, E. M., Burbidge, G. R., Fowler, W. A., & Hoyle, F. 1957, Rev. Mod. Phys., 29, 547 1.1, 1.3.2


Busso, M., Gallino, R., & Wasserburg, G. J. 1999, Annual Review of Astronomy and Astrophysics, 37, 239 1.2.2, 1.2.2, 1.3.3, 1.7, 1.3.3


Church, R. & Cristallo, S. 2009, Publications of the . . . , 1 1.5


Cristallo, S., Piersanti, L., Straniero, O., Gallino, R., Domínguez, I., Abia, C., Di Rico, G., Quintini, M., & Bisterzo, S. 2011, ApJs, 197, 17 1.5, 3.3.1, 3.3.1

Cristallo, S., Straniero, O., Gallino, R., Piersanti, L., Domínguez, I., & Lederer, M. T. 2009, The Astrophysical Journal, 696, 797 1.2.2, 1.3.3, 1.5, 3.3.1

Denissenkov, P. A., Herwig, F., Truran, J. W., & Paxton, B. 2013, 1 3.1, 3.1
Herwig, F. 2000, Astronomy and Astrophysics, 360, 952 1.3.1, 1.4.2, 1.5, 2.1.1, 2.2, 3.4
—. 2005, Annual Review of Astronomy and Astrophysics, 43, 435 1.1, 1.1, 1.2.1, 1.2.1, 1.2.1, 1.2.2, 1.4, 1.2.2, 1.3.1, 1.5, 1.4.2, 1.5, 2.3, 3.1, 4.3
Herwig, F. 2013, …Systems. Volume 4: Stellar Structure and Evolution 1.4.1, 1.4.1, 1.4.1, 1.4.2
Herwig, F., Paxton, B., Uc, K., Barbara, S., Jones, S., & Bertolli, M. 2013, in prep 3.1

56
Iliadis, C. 2008, Nuclear physics of stars 1.3.1, 1.3.2, 1.3.3
Käppeler, F., Beer, H., & Wisshak, K. 1989, Reports on Progress in Physics, 52, 945 3.3.1, 3.4
Käppeler, F., Gallino, R., Bisterzo, S., & Aoki, W. 2011, Reviews of Modern Physics, 83, 157 1.6
Karakas, A. I. 2010, VizieR Online Data Catalog, 740, 31413 1.5
Kippenhahn, R. & Weigert, A. 1990, Stellar structure and evolution (Berlin: Springer) 1.2.1, 1.2.2, 1.4.1, 1.4.1, 1.4.1, 1.4.1
Larson, R. B. 2010, 1 1.4
Bibliography

Longland, R., Iliadis, C., & Karakas, a. I. 2012, Physical Review C, 85, 065809 3.4
Mattsson, L. & Höfner, S. 2011, Astronomy and Astrophysics, 533, A42 2.3
McWilliam, A. 1997, Annual Review of Astronomy and Astrophysics, 35, 503 1.1, 1.3.3
Pignatari, M., Gallino, R., Straniero, O., & Davis, A. 2004, 75, 729 3.5
Pignatari, M., Herwig, F., Hirschi, R., Bennett, M., Rockefeller, G., & Fryer, C. 2013, 1 1.4.2, 1.5, 2.1.2, 2.1.3, 2.2, 2.3, 2.3, 2.3, 2.4, 2.6, 3.1, 3.2, 3.5, 3.5, 3.14, 4
Reifarth, R., Glorius, J., Langer, C., Meusel, O., Plag, R., Pohl, M., Schmitt, S., Sonnabend, K., & Heil, M. 2011, 1 1.3.2, 4
Reimers, D. 1975, Mem. Soc. Sci. Liege, 8, 369 2.3
Rolfs, C. E. & Rodney, W. 2005, Cauldrons in the cosmos 1.3.2, 1.3.2
Siess, L. 2010, Astronomy and Astrophysics, 512, A10 1.2.2, 2.3
Straniero, O., Gallino, R., & Cristallo, S. 2006, Nuclear Physics A, 777, 311 3.5

Sweigart, A. 1998, IAU Symposium 2.4

Thomas, B. 2013, Master’s thesis, Goethe University Frankfurt, Germany 3.5


Ventura, P., Di Criscienzo, M., Carini, R., & D’Antona, F. 2013, Monthly Notices of the Royal Astronomical Society, 431, 3642 1.2.2, 1.5, 3.1, 3.2, 3.3.2

Weiss, a. & Ferguson, J. W. 2009, Astronomy and Astrophysics, 508, 1343 2.1.1
Appendix A

Appendix

A.1 Production factor tables

In the following, as mentioned in section 3.2, a brief overview of calculated production factors is given. Isotopic production factors are shown in tables A.1 and A.2 while the elemental production factors can be found in the tables A.3 and A.4.

Table A.1: Production factors of nine stable isotopes for all star masses with \( Z = 6 \cdot 10^{-3} \).

<table>
<thead>
<tr>
<th>specie</th>
<th>1.0 Msun</th>
<th>1.65 Msun</th>
<th>2.0 Msun</th>
<th>3.0 Msun</th>
<th>4.0 Msun</th>
<th>5.0 Msun</th>
<th>6.0 Msun</th>
<th>7.0 Msun</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-2</td>
<td>5.504E-01</td>
<td>2.961E-01</td>
<td>2.309E-01</td>
<td>1.494E-01</td>
<td>3.932E-02</td>
<td>2.507E-02</td>
<td>3.428E-02</td>
<td>6.041E-02</td>
</tr>
<tr>
<td>He-3</td>
<td>7.986E+00</td>
<td>8.073E+00</td>
<td>6.153E+00</td>
<td>3.234E+00</td>
<td>1.494E+00</td>
<td>1.325E+00</td>
<td>1.063E+00</td>
<td>9.775E-01</td>
</tr>
<tr>
<td>He-4</td>
<td>1.074E+00</td>
<td>1.067E+00</td>
<td>1.092E+00</td>
<td>1.090E+00</td>
<td>1.202E+00</td>
<td>1.325E+00</td>
<td>1.400E+00</td>
<td>1.446E+00</td>
</tr>
<tr>
<td>Li-7</td>
<td>5.548E-01</td>
<td>4.442E-01</td>
<td>4.414E-01</td>
<td>2.037E-01</td>
<td>4.272E-01</td>
<td>2.006E+00</td>
<td>5.140E-01</td>
<td>1.099E-01</td>
</tr>
<tr>
<td>B-11</td>
<td>9.972E-01</td>
<td>9.999E-01</td>
<td>9.999E-01</td>
<td>1.000E+00</td>
<td>9.999E-01</td>
<td>1.000E+00</td>
<td>9.999E-01</td>
<td>9.968E-01</td>
</tr>
<tr>
<td>C-12</td>
<td>8.310E-01</td>
<td>1.258E+00</td>
<td>1.718E+01</td>
<td>1.077E+01</td>
<td>3.832E+00</td>
<td>8.426E-01</td>
<td>1.309E+00</td>
<td>7.883E-01</td>
</tr>
<tr>
<td>C-13</td>
<td>7.334E+00</td>
<td>7.329E+00</td>
<td>7.253E+00</td>
<td>7.247E+00</td>
<td>8.662E+00</td>
<td>9.736E+00</td>
<td>2.177E+01</td>
<td>2.736E+01</td>
</tr>
<tr>
<td>N-14</td>
<td>3.044E+00</td>
<td>5.910E+00</td>
<td>8.913E+00</td>
<td>1.164E+01</td>
<td>1.431E+01</td>
<td>1.866E+01</td>
<td>2.277E+01</td>
<td>2.208E+01</td>
</tr>
</tbody>
</table>
Table A.2: Production factors of nine stable isotopes for all star masses with $Z = 1 \cdot 10^{-4}$.

<table>
<thead>
<tr>
<th>specie</th>
<th>1.0 Msun</th>
<th>1.65 Msun</th>
<th>2.0 Msun</th>
<th>3.0 Msun</th>
<th>4.0 Msun</th>
<th>5.0 Msun</th>
<th>6.0 Msun</th>
<th>7.0 Msun</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-2</td>
<td>3.718E-01</td>
<td>1.895E-01</td>
<td>1.600E-01</td>
<td>3.762E-02</td>
<td>1.689E-02</td>
<td>1.243E-02</td>
<td>4.166E-02</td>
<td>4.640E-02</td>
</tr>
<tr>
<td>He-3</td>
<td>5.661E+00</td>
<td>4.873E+00</td>
<td>4.602E+00</td>
<td>2.947E+00</td>
<td>1.498E+00</td>
<td>1.009E+00</td>
<td>9.084E+00</td>
<td>7.887E+00</td>
</tr>
<tr>
<td>He-4</td>
<td>9.774E-01</td>
<td>1.118E+00</td>
<td>1.079E+00</td>
<td>1.148E+00</td>
<td>1.349E+00</td>
<td>1.566E+00</td>
<td>1.501E+00</td>
<td>1.540E+00</td>
</tr>
<tr>
<td>Li-7</td>
<td>2.245E+00</td>
<td>1.401E+00</td>
<td>1.088E+00</td>
<td>1.093E+00</td>
<td>2.081E+00</td>
<td>1.743E+00</td>
<td>8.148E+00</td>
<td>5.172E+00</td>
</tr>
<tr>
<td>B-11</td>
<td>9.220E-01</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
</tr>
<tr>
<td>C-12</td>
<td>6.698E-01</td>
<td>1.015E+03</td>
<td>1.410E+01</td>
<td>1.906E+02</td>
<td>2.343E+02</td>
<td>6.874E+00</td>
<td>6.109E+00</td>
<td>3.595E+00</td>
</tr>
<tr>
<td>Li-7</td>
<td>5.661E+00</td>
<td>4.873E+00</td>
<td>4.602E+00</td>
<td>2.947E+00</td>
<td>1.498E+00</td>
<td>1.009E+00</td>
<td>9.084E+00</td>
<td>7.887E+00</td>
</tr>
<tr>
<td>C-13</td>
<td>6.856E+00</td>
<td>2.054E+01</td>
<td>1.740E+01</td>
<td>1.906E+02</td>
<td>2.948E+02</td>
<td>1.506E+03</td>
<td>7.887E+00</td>
<td>5.172E+00</td>
</tr>
<tr>
<td>N-14</td>
<td>5.974E+00</td>
<td>3.121E+01</td>
<td>2.712E+01</td>
<td>1.770E+02</td>
<td>2.548E+02</td>
<td>1.354E+03</td>
<td>7.887E+00</td>
<td>5.172E+00</td>
</tr>
</tbody>
</table>

Table A.3: Production factors of nine stable elements for all star masses with $Z = 6 \cdot 10^{-3}$.

<table>
<thead>
<tr>
<th>specie</th>
<th>1.0 Msun</th>
<th>1.65 Msun</th>
<th>2.0 Msun</th>
<th>3.0 Msun</th>
<th>4.0 Msun</th>
<th>5.0 Msun</th>
<th>6.0 Msun</th>
<th>7.0 Msun</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>1.075E+00</td>
<td>1.068E+00</td>
<td>1.092E+00</td>
<td>1.090E+00</td>
<td>1.202E+00</td>
<td>1.325E+00</td>
<td>1.400E+00</td>
<td>1.446E+00</td>
</tr>
<tr>
<td>Li</td>
<td>5.548E-01</td>
<td>4.414E-01</td>
<td>2.037E-01</td>
<td>2.472E-01</td>
<td>2.006E+00</td>
<td>5.140E-01</td>
<td>5.140E-01</td>
<td>5.140E-01</td>
</tr>
<tr>
<td>B</td>
<td>9.973E-01</td>
<td>1.041E+00</td>
<td>1.088E+00</td>
<td>1.093E+00</td>
<td>1.202E+00</td>
<td>1.325E+00</td>
<td>1.400E+00</td>
<td>1.446E+00</td>
</tr>
<tr>
<td>C</td>
<td>8.543E-01</td>
<td>1.274E+00</td>
<td>1.695E+01</td>
<td>1.064E+01</td>
<td>3.817E+00</td>
<td>2.006E+00</td>
<td>1.000E+00</td>
<td>1.000E+00</td>
</tr>
<tr>
<td>N</td>
<td>1.303E+00</td>
<td>1.157E+00</td>
<td>1.092E+00</td>
<td>1.090E+00</td>
<td>1.202E+00</td>
<td>1.325E+00</td>
<td>1.400E+00</td>
<td>1.446E+00</td>
</tr>
<tr>
<td>O</td>
<td>9.968E-01</td>
<td>4.456E+01</td>
<td>1.005E+00</td>
<td>1.019E+00</td>
<td>1.096E+00</td>
<td>1.470E+00</td>
<td>1.580E+00</td>
<td>3.300E+00</td>
</tr>
<tr>
<td>Ne</td>
<td>9.972E-01</td>
<td>1.021E+00</td>
<td>1.722E+00</td>
<td>1.170E+00</td>
<td>1.137E+00</td>
<td>1.108E+00</td>
<td>1.018E+00</td>
<td>1.062E+00</td>
</tr>
</tbody>
</table>

Table A.4: Production factors of nine stable elements for all star masses with $Z = 1 \cdot 10^{-4}$.

<table>
<thead>
<tr>
<th>specie</th>
<th>1.0 Msun</th>
<th>1.65 Msun</th>
<th>2.0 Msun</th>
<th>3.0 Msun</th>
<th>4.0 Msun</th>
<th>5.0 Msun</th>
<th>6.0 Msun</th>
<th>7.0 Msun</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>9.782E-01</td>
<td>1.119E+00</td>
<td>1.079E+00</td>
<td>1.148E+00</td>
<td>1.349E+00</td>
<td>1.456E+00</td>
<td>1.501E+00</td>
<td>1.540E+00</td>
</tr>
<tr>
<td>Li</td>
<td>2.245E+01</td>
<td>1.401E+01</td>
<td>1.088E+01</td>
<td>1.093E+02</td>
<td>2.081E+02</td>
<td>1.743E+02</td>
<td>8.148E+00</td>
<td>5.172E+00</td>
</tr>
<tr>
<td>B</td>
<td>1.346E+00</td>
<td>3.581E+00</td>
<td>4.080E+00</td>
<td>3.231E+02</td>
<td>6.090E+02</td>
<td>8.134E+02</td>
<td>3.606E+02</td>
<td>3.517E+02</td>
</tr>
<tr>
<td>C</td>
<td>6.931E-01</td>
<td>3.189E+00</td>
<td>3.892E+00</td>
<td>3.252E+02</td>
<td>2.403E+02</td>
<td>7.261E+02</td>
<td>2.506E+02</td>
<td>9.681E+01</td>
</tr>
<tr>
<td>N</td>
<td>1.676E+00</td>
<td>4.273E+01</td>
<td>1.905E+02</td>
<td>1.019E+02</td>
<td>6.785E+01</td>
<td>3.965E+01</td>
<td>1.858E+01</td>
<td>5.020E+01</td>
</tr>
<tr>
<td>O</td>
<td>8.923E-01</td>
<td>4.565E+01</td>
<td>1.905E+02</td>
<td>1.746E+01</td>
<td>1.906E+00</td>
<td>1.470E+00</td>
<td>1.580E+00</td>
<td>4.940E+00</td>
</tr>
<tr>
<td>F</td>
<td>9.220E-01</td>
<td>1.646E+00</td>
<td>2.311E+00</td>
<td>1.007E+00</td>
<td>9.975E-01</td>
<td>9.991E-01</td>
<td>9.996E-01</td>
<td>1.001E+01</td>
</tr>
<tr>
<td>Ne</td>
<td>9.194E-01</td>
<td>4.554E+01</td>
<td>1.150E+02</td>
<td>8.966E+00</td>
<td>1.380E+01</td>
<td>1.829E+00</td>
<td>1.872E+00</td>
<td>4.895E+00</td>
</tr>
</tbody>
</table>
Authenticity declaration

I declare that *Stellar evolution, nucleosynthesis and s-process in low metallicity AGB stars* is my own work, that it has not been submitted for any degree or examination in any other university, and that all the sources I have used or quoted have been indicated and acknowledged by complete references.

Full name.................................... Date..................................
Signed........................................

A.1 Production factor tables
I would like to thank Prof. Dr. René Reifarth for offering the opportunity and support for this work. The experience I gained during that time is priceless. I appreciate the freedom I had to choose project topic.

Without Prof. Dr. Falk Herwig this thesis would not be possible. His close mentoring and guidance has lead me to a new experience. Especially the introduction to the NuGrid collaboration and their programs were an essential part and opened my eyes for different fields of astrophysics. I am looking forward to working with him in the future.

Also I would like to thank my colleagues Dr. Jan Glorius, PhD student Alexander Koloczek as well as PhD student Benedikt Thomas for the nice time together. They were always very supportive and helpful. Furthermore I am thankful for advices of various kinds by PhD student Stefan Schmidt. It was wonderful to work in such a nice research group. Thank you.

I dedicate my work to my parents and grandparents who always support and encourage me to go my path of life. Without them I would never have achieved my goals.