Nuclear reaction rates and opacity in massive star evolution calculations

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Abstract. Nuclear reaction rates and opacity are important parameters in stellar evolution. The input physics in a stellar evolution code determines the main theoretical characteristics of the stellar structure, evolution and nucleosynthesis of a star. For different input physics, in this work we calculate stellar evolution models of very massive first stars during the hydrogen and helium burning phases. We have considered 100 and 200\(M_\odot\) galactic and pregalactic stars with metallicity \(Z = 10^{-6}\) and \(10^{-9}\), respectively. The results show important differences from old to new formulations for the opacity and nuclear reaction rates, in particular the evolutionary tracks are significantly affected, that indicates the importance of using up to date and reliable input physics. The triple alpha reaction activates sooner for pregalactic than for galactic stars.

1. Introduction

The first stars provided the initial heavy elements enrichment of the intergalactic medium (IGM). Massive primordial stars marked the first step in the chemical evolution of the universe. The abundance of the CNO elements are fundamental, they form the bulk of the heavy elements with important roles in stellar interior opacities, and energy generation, affecting the star’s lifetime, evolutionary track on the HD diagram, and heavy element yields.

Two major factors that affect the nucleosynthetic yields are the \(^{12}\text{C}(\alpha, \gamma)^{16}\text{O}\) reaction rate and the efficiency of semiconvective mixing (Weaver and Woosley 1993). The evaluation of the cross-section for the different nuclear burning processes is required for establishing the energy balance of the star. Many cross-sections are known with high accuracy. However, there are uncertainties with some important processes for both hydrogen, and helium burning, where nuclear rates are not well known (Cassisi 2005). The radiative opacity is related to the mean free path of the photons and it is very important in determining the efficiency of heat transfer via radiative processes.

Nuclear reaction rates and opacities have been changing with time. In this paper, we calculate models of very massive first stars with the aim of comparing their evolutionary tracks by using different old and new formulations for the opacity and nuclear reaction rates.

In Section 2 we present a brief review concerning nuclear reaction rates. In Section 3, the same for the opacity as well. In Section 4 some results are described, and in Section 5 we discuss the importance of the input physics, specifically nuclear physics, and outline some conclusions.
2. Nuclear reaction rates

2.1. Nuclear reactions in astrophysics

Nuclear processes in massive stars have been proposed as the source of most of the isotopes heavier than helium now present in the universe. Stellar evolution models incorporate detailed nuclear reaction networks based on accurate calculations or measurements of nuclear cross-sections.

A first review of the available experimental data on cross-sections for the nuclear interactions of neutrons, protons, and alpha particles with a number of light and intermediate-mass nuclei was made by Fowler, Caughlan and Zimmermann (1967).

Stellar thermnuclear reaction rates were revised and updated by Fowler, Caughlan and Zimmermann (1975), and Harris et al (1983) adding new laboratory measurements of nuclear cross-sections. Furthermore, new data were included by Caughlan et al (1985), and Caughlan and Fowler (1988).

Remarkable progress have been made in reaction rates at energies close to those of astrophysical relevance (Rolfs and Rodney 1988). Despite these efforts, important uncertainties remain.

The Nuclear Astrophysics Compilation of Reaction Rates (NACRE) have documented and evaluated sets of experimental data or theoretical predictions for a large number of astrophysical nuclear reactions (Angulo, Arnould and Rayer 1999). This compilation included the rates for all the charged-particle-induced reactions involved in the pp, CNO, NeNa and MgAl chains. The first two chains are energy producers but all four are important nucleosynthesis agents. Non-explosive He-burning reactions were also included.

2.2. Evolutionary calculations

The abundances of the isotopes from C to Al produced by the non-explosive CNO, NeNa and MgAl modes of hydrogen burning, as well as by helium burning were calculated by Arnould, Goriely and Jorissen (1999) using the NACRE thermonuclear rates.

In their evolutionary calculations of zero-metallicity stars, Marigo et al (2001) evaluated the changes in chemical abundances due to nuclear reactions by solving a network consisting of a set of reactions for the pp1 chain, the CNO tri-cycle and the most important α-capture reactions. The reaction rates are from Caughlan and Fowler (1988) compilation, except for $^{17}\text{O}(p,\alpha)^{14}\text{N}$ and $^{17}\text{O}(p,\gamma)^{18}\text{F}$, for which they used determinations by Landré et al (1990).

To study the cosmological effects of the first stars, Tumlinson, Shull and Venkatesan (2003) considered a nuclear reaction network coupled to the stellar structure equations. The network includes the relevant nuclear reactions for 24 isotopic abundances. The reaction rates are from Caughlan and Fowler (1988) compilation.

A nuclear network following the evolution of 13 isotopes was implemented by Claret (2004) for the pp-chains, CNO tri-cycle, helium and carbon burning reactions. The basic nuclear reactions are from Caughlan and Fowler (1988), while the screening factors are taken from Graboske et al (1973). In the new grids of stellar models from Claret (2005) all reaction rates are taken from NACRE with the exception of the $^{14}\text{N}(p,\gamma)^{15}\text{O}$ reaction, for which a new rate has been implemented (Runkle 2003, Formicola et al. 2004). This reaction is the slowest step of the CNO cycle and the effect on the evolutionary life of the stars will depend on the stellar mass.

The reliability of theoretical predictions of the evolutionary lifetime depends on the accuracy of the nuclear reaction rates since nuclear burning provides the bulk of the stellar luminosity during the main evolutionary phases (Cassisi 2005).

For calculating their first stars structure and evolution models, Bahena and Klapp (2010) used the NACRE compilation of nuclear reaction rates.
3. Radiative opacities

3.1. Tabulated opacities

The calculation of realistic stellar opacities is among the most difficult problem in stellar astrophysics. At the present time, the most commonly used opacities for stellar mixtures are those generated at the Los Alamos National Laboratory (LANL) and at the Lawrence Livermore National Laboratory. Opacities are available in tabular form and include many stellar mixtures with opacities computed over a wide density and temperature range.

In practice, extensive tables or, sometimes, an analytic fit to the tables are used that gives radiative and conductive opacities over a wide temperature and density range for the various compositions of interest. A specific opacity is obtained by a multidimensional interpolation between the tables. For a decades, the Cox and Stewart (1965, 1970a, 1970b) opacity tables were used as standard. To recompute new opacity tables, two major independent efforts were made. One was the Opacity Project (Seaton 1987, Berrington et al 1987), and the other one is known as OPAL.

The Rosseland mean opacity tables calculated with the OPAL code for various compositions over a wide range of densities and temperatures for typical stellar conditions were presented by Rogers and Iglesias (1992). The OPAL code removes several approximations in the equation of state and atomic data generation present in past calculations. A comparison to Eggleton, Faulkner and Flannery (1973) produces small differences. OPAL results allow accurate interpolation in temperature, density, hydrogen mass fraction, as well as metal mass fraction. The tables do not include atmospheric and high-temperature opacities, only radiation processes are taken into account.

Iglesias and Rogers (1991), and Rogers and Iglesias (1992) demonstrated that the inclusion of more metal lines that were previously considered can greatly increase the total opacity at temperatures above $10^9$ K. Further refinements of the atomic physics were incorporated into the OPAL opacity code. The tables were extended to lower and higher densities as well as higher metallicity (Iglesias, Rogers and Wilson 1992).

3.2. Opacity for massive stars

One of the major problems in working with very massive stars is that a quasi-static stellar evolution code very easily becomes unstable. The problem becomes worse as the mass of the star is increased and in many cases it is very difficult to find out what is causing the instabilities. The use of opacity tables contribute to make the code unstable.

During many years the opacity was obtained by interpolating from Cox-Stewart opacity tables. The way in which the interpolation is done causes the opacity to oscillate slightly as you move from the vicinity of one table point to another. It is this small variation in the opacity which makes the code unstable, which also shows how sensitive very massive star calculations are to the programming input physics. In view of this difficulty it is convenient to use Christy’s (1966) analytic fit to the tables which can be written as

$$
\kappa = P_e \left[5.4 \times 10^{-13} \rho^{-1} T_4^{-1} \left(1/(1 + 2T_9)\right)\right] + XT_4^{1/2} \left(2 \times 10^6 T_4^{-4} + 2.1 T_4^{-6}\right)^{-1} + X \left\{4.5 T_4^5 + T_4^{-1} \left(4 \times 10^{-3} T_4^{-1} + 2 \times 10^{-4} \rho^{-1/4}\right)^{-1}\right\}^{-1} + Y \left\{(1.4 \times 10^3 T_4 + T_4^{5/2})^{-1} + 1.5(10^6 + 0.1 T_4^4)^{-1}\right\}^{-1} \left\{1 - X - Y\right\} \left\{T_4^{1/2} + (20 T_4 + 5 T_4^2 + T_4^5)^{-1}\right\}^{-1}
$$

(1)

where $T$ is the temperature, $P_e$ the electron pressure, and the first term has been modified to take into account the Klein-Nishina contribution to the opacity (Klapp 1982, 1983). The first
term gives the free-electron scattering contribution, the second is due to hydrogen, the third to helium, and the last one to heavy elements.

For very massive stars most of the instabilities disappear with the use of equation (1), which has been used by Klapp (1982, 1983, 1984), Klapp et al (2005, 2006), Bahena (2006), and Bahena, Klapp and Dehnen (2007).

3.3. Evolutionary models
The computation of new opacity tables was performed by the Geneva group with the Los Alamos opacity programme (Maeder 1990).

The new stellar opacities are found to lead to revised evolutionary models for stars from intermediate to high masses. With the use of these opacities a remarkably close agreement with observed stars was obtained (Stothings and Chin 1991). Claret and Giménez (1991) used opacities based in the latest calculations from Los Alamos. The chemical composition adopted corresponded to Population I. The new opacities obtained at Lawrence Livermore National Laboratory by Rogers and Iglesias (1992) were introduced by Claret and Giménez (1992) together with the Los Alamos Astrophysical Opacity Library (LAOL) (Huebner et al 1977, Weiss, Keady and Magee 1990).

Schaller et al (1992) presented new grids of stellar models at various metallicities using the tables of Huebner et al (1977), the opacities by Rogers and Iglesias (1992) and by Kurucz (1991) at low temperature. Charbonnel et al (1993), and Schaerer (1993a, 1993b) also used the OPAL radiative opacities (Iglesias, Rogers and Wilson 1992). Claret (1995) adopted the OPAL opacities and Los Alamos tables. Claret (2004, 2005) adopted in his models the radiative opacities by Iglesias and Rogers (1996) for higher temperatures, complemented with Alexander and Ferguson (1994) results for lower temperatures.

The radiative opacities from the OPAL group (Rogers and Iglesias 1992, Iglesias and Rogers 1993) were used by Marigo et al (2001). The conductive opacities for electron-degenerate matter were from Hubbard and Lampe (1969). In the domain of high temperatures, Siess, Livio and Lattanzio (2002) used the OPAL opacity tables and other opacities computed by several authors.

For a 300 $M_{\odot}$ star, Bromm, Kudritzki and Loeb (2001) considered that the only source of opacity is electron scattering and used the well known expression $\kappa = 0.20(1+ X) \text{ cm}^2 \text{ g}^{-1}$. The Rosseland mean opacity from the OPAL tables (Iglesias and Rogers 1996) have been used by Tumlinson, Shull and Venkatesan (2003) to calculate their models for very massive first stars.

For the structure and evolution models of the first stars, Bahena and Klapp (2010) used the opacities from the OPAL group.

4. Results

4.1. Initial conditions
For this work we calculated models for 100 and 200 $M_{\odot}$ galactic and pregalactic Population III stars, and two different chemical compositions which are the following: $(X, Z) = (0.765, 10^{-6})$, and $(X, Z) = (0.765, 10^{-9})$, for galactic and pregalactic Population III stars, respectively.

4.2. Code and input physics
The system of stellar structure and evolution equations used in the numerical code has been described by Klapp (1982, 1983) and Klapp et al. (2005, 2006). Concerning input physics, in this work we consider three cases: a) nuclear reaction rates from Harris et al (1983), and an analytic opacity formulation from Christy (1966); b) nuclear reaction rates from Harris et al (1983), and opacities from Rogers and Iglesias (1992) and Iglesias and Rogers (1993, 1996); c) the NACRE compilation from Angulo, Arnould and Rayer (1999) and opacities from the OPAL group. Evolutionary calculations have been made without mass loss and no rotation, during the hydrogen and helium burning phases.
Figure 1. Evolutionary tracks in the HR-diagram for 100 and 200\(M_\odot\) galactic stars with metallicity \(Z = 10^{-6}\) during the hydrogen, and helium burning phases.

### 4.3. Evolutionary tracks

Figures 1 and 2 show the evolutionary tracks in the Hertzsprung-Russell (HR) diagram for 100 and 200\(M_\odot\) galactic and pregalactic Population III stars, respectively, with different input physics during the hydrogen and helium burning phases.

Massive star evolutionary tracks during the hydrogen and helium burning phases are characterized by a continuous movement to the right of the HR-diagram, describing different paths depending on the stellar mass and the mass loss rate.

In the HR-diagram the locus of very massive Population III stars is in the left upper part. Pregalactic stars are hotter than galactic ones. Stars with lower metallicity are shifted to the left because they are bluer than the others.

The most massive stars are very hot and luminous. Luminosity decreases with lower metallicity. Stars settle down on the main sequence with a high effective temperature and luminosity. During hydrogen burning all stars increase their luminosity while a helium mass fraction is formed. The central density and temperature both increases. At the end of hydrogen burning a transition to helium burning takes place.

For galactic stars the transition to helium burning is accompanied with an explosive event and the contraction of the star. For pregalactic stars, this transition occurs very smoothly because they are hotter and their central temperature is high enough to ignite helium promptly.

The hydrogen and helium burning phases takes place at the blue side of the HR-diagram. When stars evolve they move towards the red and without mass loss they do not experience the asymptotic giant branch (AGB).
Figure 2. Evolutionary tracks in the HR-diagram for 100 and 200\( M_\odot \) pregalactic stars with metallicity \( Z = 10^{-9} \) during the hydrogen, and helium burning phases.

Comparing the three studied cases for 100 and 200\( M_\odot \) galactic stars we observe the following: for case (a) (old opacity and old rates), stars are hotter and more luminous than for case (c) (new opacities and new rates) during the hydrogen and helium burning phases, and stars evolving without mass loss never reach the AGB. For case (b) (new opacities and old rates), stars evolve with lower effective temperature and luminosity than for case (a) during hydrogen burning, but similarly for helium burning.

For pregalactic stars of the same mass, the behavior is similar to galactic ones with the difference that stars are hotter and slightly less luminous than for the galactic case.

Theoretical analysis predict the final fate of massive stars. If the first generation of stars have been quite massive (100 – 300\( M_\odot \)), and retain their high mass until death, such stars will make pair-instability supernovae (PISNe) (Fryer, Woosley and Heger (2001). This is the main characteristic of these stars.

Heger and Woosley (2002) have explored helium cores nucleosynthesis in the mass range \( M_{\text{He}} = 64 – 130M_\odot \), corresponding to main sequence masses of approximately 140 – 260\( M_\odot \). They suggest different scenarios. The ultimate fate of a metal-free star depends critically on its mass. PISNe nucleosynthesis varies greatly with the helium core mass.

In our models, the stars develop large convective cores. The PISNe scenario and hypernovae (HNe) hypothesis have been discussed by Klapp and Bahena (2008).

The nucleosynthesis constrains on a pregalactic generation of stars has been studied by Abia et al (2001). They found that the possible contribution of the Population III remnants to the baryonic dark matter is insignificant.
It is often suggested that the initial heavy element enrichment is due to the first generation of stars. In our very massive models, the most abundant nuclei produced during hydrogen burning nucleosynthesis is $^{14}$N (Bahena, Klapp and Dehnen 2007).

5. Discussion and conclusions

From the comparison of the evolution of very massive Population III stars using different opacities and nuclear reaction rates we found that the evolutionary tracks in the HR-diagram are similar. Pregalactic stars are hotter than galactic ones because the triple alpha reaction actives sooner during hydrogen burning.

However, there exist differences in the effective temperature and luminosity for the old and new values. The best results are obtained for the later case.

This shows that the input physics is very important in stellar evolution calculations. Different opacities and/or nuclear reaction rates yield different evolutionary tracks.

Uncertainties in several reaction rates still exist, such as the triple alpha reaction and the $^{12}$C($\alpha$, $\gamma$)$^{16}$O reaction. For this reaction NACRE considers a factor of 2 to be the uncertainty in the reaction rate, responsible for the $^{16}$O abundance.

This reaction has a significant influence on massive star advanced stages of evolution. Heger \textit{et al} (2002) have studied the nucleosynthesis and nuclear reaction uncertainties for massive star evolution. They consider that the uncertain $^{12}$C($\alpha$, $\gamma$)$^{16}$O reaction rate has a significant influence on advanced massive star evolution, and also determines whether a neutron star or black hole is formed.

For the critically important $^{12}$C($\alpha$, $\gamma$)$^{16}$O reaction, the cross-section used by Weaver and Woosley (1993), Woosley and Weaver (1995), and Woosley, Langer and Weaver (1993) has been 1.7 times the value given at each temperature by Caughlan and Fowler (1988). In their pre-supernova evolution and supernova explosion calculations, Umeda, Nomoto and Nakamura (2000) have chosen a value which is 1.4 times that given by Caughlan and Fowler (1988). Heger \textit{et al} (2002) used a value which is 1.2 times the $^{12}$C($\alpha$, $\gamma$)$^{16}$O rate of Buchmann (1996).

In Marigo \textit{et al} (2001) the uncertain $^{12}$C($\alpha$, $\gamma$)$^{16}$O rate was set to 1.7 times the value given by Caughlan and Fowler (1988) and Weaver and Woosley (1993) for a massive star nucleosynthesis calculation, with electron screening factors for all reactions taken from Graboske \textit{et al} (1973).

The $^{12}$C($\alpha$, $\gamma$)$^{16}$O and $^4$He(2$\alpha$, $\gamma$)$^{12}$C reactions compete for helium consumption, and thus the relative rate of these reactions determine whether oxygen or carbon is the dominant helium burning product. The triple alpha reaction rate is crucial for the first stars evolution but its rate is still under discussion.

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References

Abia C, Domínguez I, Straniero O, Limongi M, Chieffi A and Isern J 2001 \textit{ApJ} \textbf{557}, 126
Alexander D R and Ferguson J W 1994 \textit{ApJ} \textbf{437} 879
Angulo C, Arnould M, Rayer M \textit{et al} 1999 \textit{Nucl. Phys. A} \textbf{656} 3
Arnould M, Goriely S and Jorissen A 1999 \textit{A&A} \textbf{347} 572
Bahena D 2006 \textit{PhD Thesis} Univerzita Karlova v Praze
Bahena D, Klapp J and Dehnen H 2007 \textit{Rev. Mex. Fís} \textbf{53}, 48
Bahena D and Klapp J 2010 \textit{ApSS} \textbf{327}, 219
Berrington K A, Burke P G, Butler K \textit{et al} 1987 \textit{J. Phys. B: Al. Mol. Phys.} \textbf{20} 6369
Bromm V, Kudritzki R P and Loeb A 2001 \textit{ApJ} \textbf{552} 464
Buchmann L 1996 ApJL 468 127
Cassisi S 2005 [arXiv: astro-ph/0506161
Caughlan G R and Fowler 1988 At. Data Nucl. Data Tables 40 283
Caughlan G R, Fowler W A, Harris M J and Zimmerman B A 1985 At. Data Nucl. Data Tables 32 197
Charbonnel C, Meynet G, Maeder A, Schaller G and Schaerer D 1993 A&AS 101 415
Christy R 1966 ApJ 144 108
Claret A 1995 A&AS 109 441
Claret A 2004 A&AS 142 419
Claret A 2005 A&AS 440 647
Claret A and Giménez A 1991 A&AS 87 507
Claret A and Giménez A 1992 A&AS 96 255
Cox A N and Steward J N 1965 ApJS 11 22
Cox A N and Steward J N 1970a ApJS 19 243
Cox A N and Steward J N 1970b ApJS 19 261
Fowler W A, Caughlan G and Zimmerman B A 1967 ApJ 5 525
Fowler W A, Caughlan G and Zimmerman B A 1975 ApJ 13 69
Fryer C L, Woosley S E and Heger A 2001 ApJ 550 372
Formicola A et al 2004 Phys. Lett. B 591 61
Graboske H C, DeWitt H L, Grossman A S and Cooper M S 1973 ApJ 181 457
Harris M J, Fowler W A, Caughlan G and Zimmerman B A 1983 ARA&A 21 165
Heger A and Woosley S E 2002 ApJ 567 532
Heger A, Woosley S E, Rauscher T, Hoffman R D and Boyes M M 2002 New Astron. Rev. 46 463
Hubbard W B and Lampe M E 1969 ApJS 18 297
Huebner W F, Merts A L, Magee N H and Argo M F 1977 Los Alamos Scientific Report, LA-6760-M
Iglesias C A and Rogers F J 1991 ApJS 371 408
Iglesias C A and Rogers F J 1993 ApJS 412 752
Iglesias C A and Rogers F J 1996 ApJS 464 943
Iglesias C A, Rogers F J and Wilson B G 1992 ApJ 397 717
Klapp J 1983 ApSS 99 313
Klapp J 1984 ApSS 106 215
Klapp J and Bahena D 2008 Rev. Mex. Fís S 54 74
Klapp J, Bahena D, Corona-Galindo M G and Dehnen H 2005 in Gravitation and Cosmology, eds. A Macías, C. Lämmerzahl and D Nuñez, Melville N Y, AIP Conf. Proc. 758 153
Klapp J, Bahena D, Corona-Galindo M G, Dehnen H and Galindo S 2006 Rev. Mex Fis. 52 50
Kurucz R L 1991 in Stellar Atmospheres: Beyond Classical Models, NATO ASI Series C, 341
Landré V, Prandtznos N, Aguer P et al 1990 A&A 240 85
Maeder A 1990 A&AS 84 139
Marigo P, Girardi L, Chiosi C and Wood P R 2001 A&A 347 152
Rogers F J and Iglesias C A 1992 ApJS 79 507
Rols C E and Rodney W S 1988 Cauldrons in the Cosmos, University of Chicago
Runke R C 2003 PhD Thesis, University of North Carolina
Seaton M J 1987 J. Phys. B: At. Mol. Phys. 20 6363
Schauer D, Meynet G, Maeder A and Schaller G 1993a A&AS 98 523
Schauer D, Charbonnel C, Meynet G, Maeder A and Schaller G 1993b A&AS 102 339
Schaller G, Schauer D, Meynet G and Maeder A 1992 A&AS 96 269
Siess L, Livio M and Lattanzio J 2002 ApJ 570 329
Stothers R and Chin C W 1991 ApJ 381 L67
Tumlinson J, Shull J M and Venkatesan A 2003 ApJ 528 L65
Umeda H, Nomoto K and Nakamura T 2000, In The First Stars: Proceedings of the MPA/ESO Workshop Held at Garching, Germany, 4-6 August 1999, ESO Astrophysics Symposia. Edited by A. Weiss, T.G. Abel, and V. Hill. Springer-Verlag, p. 150
Weaver T A and Woosley S E 1993 Phys. Rep. 227 65
Woosley S E and Weaver T A 1995 ApJS 101 181
Woosley S E, Langer N and Weaver T A 1993 ApJ 411 823
Weiss A, Keady J J and Magee N H 1990 Atomic and Nuclear Data Tables 45 209