Evolution of AGB stars at varying surface C/O ratio: The crucial effect of molecular opacities

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Abstract. This study calls attention to the importance of properly coupling the molecular opacities to the actual surface abundances of TP-AGB stars that experience the third dredge-up and/or hot-bottom burning, i.e. with surface abundances of carbon and oxygen varying with time. New TP-AGB calculations with variable opacities – replacing the usually adopted solar-scaled opacity tables – have proven to reproduce, for the first time, basic observables of carbon stars, like their effective temperatures, C/O ratios, and near-infrared colours. Moreover, it turns out that the effect of envelope cooling – due to the increase in molecular opacities – may cause other important effects, namely: i) shortening of the C-star phase; ii) possible reduction or shut-down of the third dredge-up in low-mass carbon stars; and iii) weakening or even extinction of hot-bottom burning in intermediate-mass stars.

1. Introduction

The observed spectral dichotomy between M-type (with C/O < 1) and C-type (with C/O > 1) stars was first explained by Russell (1934) on the basis of molecular equilibria calculations. It was pointed out that the C/O ratio plays the key-role in determining the different patterns of molecular abundances, hence different dominant molecular bands, characterising the two classes of giant stars.

Despite this basic fact, the description of molecular opacities is still improper in most evolution models of AGB stars. In fact, the usually adopted opacity tables (e.g. Alexander & Ferguson 1994) are strictly valid for solar-scaled abundances of elements heavier than helium, corresponding to C/O = 0.48 (hereinafter also $\kappa_{\text{fix}}$ prescription).

Therefore, it is already clear that the inadequacy of the opacity prescription becomes particularly serious when modelling carbon stars, characterised by surface C/O > 1 as a consequence of recurrent third dredge-up episodes during the TP-AGB evolution.

Marigo (2002) investigates the effects on the AGB evolution due to variable molecular opacities (hereinafter also $\kappa_{\text{var}}$ prescription), that are now computed consistently to the current envelope chemical composition of TP-AGB models experiencing the third dredge-up and hot-bottom burning (HBB).

As illustrated in the following, from comparing the new $\kappa_{\text{var}}$ with the standard $\kappa_{\text{fix}}$ results, the impact turns out indeed significant.
Figure 1. Molecular abundances (in terms of partial pressures) of a few atomic and molecular species as a function of the C/O ratio, assuming a gas pressure $P_{\text{gas}} = 10^3$ dyne cm$^{-2}$, and a temperature $T = 2500$ K. The vertical line marks the molecular concentrations for a solar composition, with C/O $\sim 0.48$.

2. Solar-scaled vs. variable molecular opacities

A routine has been constructed to derive the molecular concentrations through dissociation equilibrium calculations, and estimate the opacities due to H$_2$, H$_2$O, OH, C$_2$, CN, and CO for any given density, temperature and chemical composition of the gas (Marigo 2002).

Figure 1 displays an example of the expected chemical pattern at increasing C/O ratio (carbon abundance is augmented, while that of oxygen is kept fixed). Note the abrupt change in the chemical abundances, as C/O increases from below to above unity, for all species but for CO molecule. In fact, most atoms of the least abundant element between C and O are trapped into the CO molecule, due to its high binding energy.

Such an abrupt change in molecular abundances at the transition from C/O $< 1$ to C/O $> 1$ results, in turn, into a drastic change in the dominant sources of molecular opacities. This is illustrated in Fig. 2, based on Marigo’s (2002) calculations (solid line). As C/O increases the H$_2$O opacity bump, preponderant as long as C/O $< 1$, progressively reduces until it completely disappears for C/O $= 1$, and finally the CN opacity bump develops as soon as C/O $> 1$. We also notice that, instead, the solar-scaled opacities (dashed line) would predict a minimum just in place of the CN bump.
Figure 2. Mass absorption coefficient as a function of the C/O ratio, based on Marigo (2002) calculations (solid lines). For comparison we also show the case of solar-scaled opacities (for $C/O \sim 0.48$) according to Alexander & Ferguson (1994) tables (dashed lines).

3. New synthetic TP-AGB models with variable molecular opacities

Synthetic TP-AGB models, based on complete envelope integrations (see Marigo et al. 1996, 1998), are computed by adopting either the new $\kappa_{\text{var}}$ routine, or Alexander & Ferguson (1994) opacity tables, the standard $\kappa_{\text{fix}}$ prescription. A number of important consequences derive from the comparison of the results.

3.1. Effective temperatures, C/O ratios, and lifetimes of C-stars

The empirical data shown in Fig. 3 clearly indicates two major facts, namely: i) the almost complete segregation in effective temperature between oxygen-rich and carbon-rich stars; and ii) the relatively low C/O values ($< 2$) measured in carbon-rich stars.

The disagreement is remarkable for $\kappa_{\text{fix}}$ models, that are characterised by too high effective temperatures and C/O ratios. New $\kappa_{\text{var}}$ models, instead, very well succeed in reproducing the observed location of both oxygen- and carbon-rich stars in the C/O vs. $T_{\text{eff}}$ diagram.

The reason resides just in the abrupt opacity change occurring at the transition from the O-rich to C-rich class, which causes the large excursion towards lower effective temperatures. This effect is not present in $\kappa_{\text{fix}}$ models.

The photospheric cooling, in turn, favours larger and larger mass-loss rates, contributing to anticipate the onset of the super-wind, hence the end of the AGB phase. This effect implies a shortening of the C-star phase, and a lowering of the typical C/O ratios because of fewer thermal pulses, hence dredge-up episodes.

We estimate that, for the same model prescriptions (i.e. dredge-up parameters
P. Marigo

Figure 3. Effective temperatures as a function of the C/O ratio in Galactic giants. Abundance determinations are taken from: Smith & Lambert (1990 and references therein) for M stars (C/O $< 1$); Ohnaka & Tsuji (1996) for S stars (C/O $\sim 1$); Lambert et al. (1986), Ohnaka et al. (2000) for C stars (C/O $> 1$). Effective temperatures are taken from the quoted works, and Bergeat et al. (2001) for C-stars and mass-loss law), the C-star lifetimes can be reduced up to a factor of 2 – 3 when adopting the variable opacities.

3.2. Effects on the third dredge-up

With the aid of envelope integrations we have explored the possible effects on the third dredge-up due to the $\kappa_{\text{var}}$ prescription. In summary it turns out that, at the stage of the post-flash luminosity maximum (corresponding to the maximum penetration of envelope convection), the envelope base temperature, $T_b$, may significantly decrease as soon as C/O $> 1$.

This fact would translate into a likely reduction of the third dredge-up efficiency, even determining a possible inhibition of further dredge-up events. In other words, besides the reduction of the envelope mass due to mass loss, another possible mechanism leading to the shut-down of the third dredge-up may be related to the envelope cooling caused by opacity effects.

Preliminary calculations (see Fig. 4) indicate that, especially at lower metallicities, low-mass TP-AGB stars may experience just one single dredge-up episode, become carbon stars, and thereafter preserve their chemical composition unchanged. It is also interesting to notice that, in case of solar metallicity low-mass stars, the freezing of the surface abundances as soon as C/O $\geq 1$ could provide a possible explanation to the formation of S-type stars. At larger masses the recurrence of dredge-up episodes could have an intermittent behaviour, the final shut-down possibly occurring at later stages.
3.3. Effects on hot-bottom burning

Our investigation is then extended to stars with larger masses, say $M > 4.5M_\odot$ (Marigo 2003, in preparation). It turns out that variable molecular opacities may significantly influence the structure and nucleosynthesis of massive AGB stars by affecting the efficiency of HBB.

Specifically, test calculations with $\kappa_{\text{var}}$ prescription (see Fig. 5) indicate that if during the early stages of its TP-AGB evolution, a massive AGB star has experienced efficient carbon dredge-up becoming a carbon star, then HBB may be significantly weakened or even prevented. The main reason is two-fold: The increase in opacities as soon as $\text{C/O} > 1$ produces a cooling of both i) the envelope base – hence lowering the nuclear reaction rates –, and ii) the surface – hence lowering $T_{\text{eff}}$ with consequent earlier attainment of larger mass-loss rates.

All these feedback effects are missed in the case of $\kappa_{\text{fix}}$ models, as we see by comparing the evolution of envelope chemical abundances presented in Fig. 5. For instance, note that at some stage the $\kappa_{\text{var}}$ model should appear as a luminous J-type carbon star (with $\text{C/O} > 1$ and $^{12}\text{C}/^{13}\text{C}$ close to the equilibrium value), whereas the $\kappa_{\text{fix}}$ model would belong to the class of luminous M-type giants.

4. Conclusions

This explorative study has shown how large is the impact of introducing variable molecular opacities in AGB models. This has improved the comparison with
Figure 5. Evolution of surface abundance ratios (elemental abundances are expressed by number, in mole g\(^{-1}\)) in the envelope of a (4.5 M\(_{\odot}\), Z = 0.004) model, suffering both the third dredge-up and HBB. Calculations are carried out over the entire TP-AGB evolution. Note that in the \(\kappa_{\text{var}}\) model, once the transition to carbon star (C/O > 1) has occurred, the C/O ratio no more decreases below unity, contrarily to the \(\kappa_{\text{fix}}\) case.

observations and brought many new results, which may critically change and revitalise, in various aspects, the present scenario of AGB evolution.

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