Derivation of mean molecular mass in terms of electron fraction

Luke Chamandy

July 27, 2020

We want to derive an expression for the mean molecular mass μ in terms of the number of free electrons per nucleon $f_{\rm e}$.

The mass fractions of hydrogen, helium and metals are given by

$$X = \frac{n_{\rm H} m_{\rm H}}{n_{\rm H} m_{\rm H} + n_{\rm He} m_{\rm He} + n_{\rm Z} m_{\rm Z}} = \frac{m_{\rm H}}{M}, \tag{1}$$

where $n_{\rm H}$, $n_{\rm He}$ and $n_{\rm Z}$ are the number densities of hydrogen, helium and metals, and

$$M \equiv m_{\rm H} + m_{\rm He} n_{\rm He}/n_{\rm H} + m_{\rm Z} n_{\rm Z}/n_{\rm H}. \tag{2}$$

Similarly,

$$Y = \frac{m_{\rm He} n_{\rm He}/n_{\rm H}}{M}, \qquad Z = \frac{m_{\rm Z} n_{\rm Z}/n_{\rm H}}{M}. \tag{3}$$

Now the mean molecular mass is given by

$$\mu = \frac{n_{\rm H} m_{\rm H} + n_{\rm He} m_{\rm He} + n_{\rm Z} m_{\rm Z}}{n_{\rm H} + n_{\rm He} + n_{\rm Z} + n_{\rm e}} = \frac{m_{\rm H} + n_{\rm He}/n_{\rm H} m_{\rm He} + n_{\rm Z}/n_{\rm H} m_{\rm Z}}{1 + n_{\rm He}/n_{\rm H} + n_{\rm Z}/n_{\rm H} + n_{\rm e}/n_{\rm H}} \tag{4}$$

where $n_{\rm e}$ is the number density of free electrons.

The free electron fraction (number of free electrons per nucleon), as outputted by the MESA tabular equation of state (EoS) is given by

$$f_{\rm e} = \frac{n_{\rm e}}{n_{\rm H} + 4n_{\rm He} + A n_{\rm Z}}, \tag{5}$$

where A is the mean number of nucleons of metals. For Solar composition, we would expect $A \approx 15.5$, and we will adopt $A = 16$. Rearranging the above equation gives

$$n_{\rm e} = (n_{\rm H} + 4n_{\rm He} + A n_{\rm Z}) f_{\rm e}. \tag{6}$$

Substituing Eq. (6) into Eq. (4) we obtain

$$\begin{aligned} \mu &= \frac{n_{\rm H} m_{\rm H} + n_{\rm He} m_{\rm He} + n_{\rm Z} m_{\rm Z}}{n_{\rm H} + n_{\rm He} + n_{\rm Z} + (n_{\rm H} + 4n_{\rm He} + A n_{\rm Z}) f_{\rm e}} = \frac{m_{\rm H} + m_{\rm He} n_{\rm He}/n_{\rm H} + m_{\rm Z} n_{\rm Z}/n_{\rm H}}{1 + f_{\rm e} + (1+4f_{\rm e}) n_{\rm He}/n_{\rm H} + (1 + A f_{\rm e}) n_{\rm Z}/n_{\rm H}} \\ &= \frac{M}{1 + f_{\rm e} + (1+4f_{\rm e}) n_{\rm He}/n_{\rm H} + (1 + A f_{\rm e}) n_{\rm Z}/n_{\rm H}}. \end{aligned} \tag{7}$$

Now rearranging Eq. (3), we find

$$\frac{n_{\rm He}}{n_{\rm H}} = \frac{MY}{m_{\rm He}} = \frac{m_{\rm H}}{m_{\rm He}}\frac{Y}{X}, \qquad \frac{n_{\rm Z}}{n_{\rm H}} = \frac{MZ}{m_{\rm Z}} = \frac{m_{\rm H}}{m_{\rm Z}}\frac{Z}{X}. \tag{8}$$

Subsituting these relations into Eq. (7), we obtain

$$\begin{aligned}\mu &= \frac{m_{\rm H}/X}{1 + f_{\rm e} + (1+4f_{\rm e})(m_{\rm H}/m_{\rm He})Y/X + (1+Af_{\rm e})(m_{\rm H}/m_{\rm Z})Z/X} \\ &= m_{\rm H}\left[(1+f_{\rm e})X + (1+4f_{\rm e})Ym_{\rm H}/m_{\rm He} + (1+Af_{\rm e})Zm_{\rm H}/m_{\rm Z}\right]^{-1}.\end{aligned} \tag{9}$$

Now, we can simplify further by putting

$$\frac{m_{\rm H}}{m_{\rm He}} \approx \frac{1}{4}, \qquad \frac{m_{\rm H}}{m_{\rm Z}} \approx \frac{1}{A}. \tag{10}$$

Then we obtain

$$\mu \simeq m_{\rm H}\left[(1+f_{\rm e})X + (1/4+f_{\rm e})Y + (1/A+f_{\rm e})Z\right]^{-1}. \tag{11}$$

But

$$Y = 1 - X - Z, \tag{12}$$

so Eq. (11) can be rewritten as

$$\mu \simeq m_{\rm H}\left[(1+f_{\rm e})X + (1/4+f_{\rm e})(1-X-Z) + (1/A+f_{\rm e})Z\right]^{-1}. \tag{13}$$

After a little algebra, we obtain our final expression

$$\mu \simeq m_{\rm H}\left[1/4 + 3X/4 - (1/4-1/A)Z + f_{\rm e}\right]^{-1}. \tag{14}$$

For the RGB profile used in our simulations (profile 88), we have $X = 0.69144$, $Z = 0.02019$, and we may use $A \approx 16$. The value of μ obtained using Eq. (14) is very close to that obtained directly from MESA output of μ. In the AstroBEAR simulation, it is assumed that $X = 0.69$ and $Z = 0.02$, with $f_{\rm e}$ outputted from the EoS tables corresponding to those values. The resulting profile for μ agrees quite closely with that of the MESA profile inside of $r \approx 45\,{\rm R}_\odot$. Outside of this, the pressure in the simulation differs from that of the MESA profile, so other parameters like μ also deviate from MESA.