R Coronae Borealis Star Evolution: Simulating 3D Merger Events to 1D Stellar Evolution Including Large-scale Nucleosynthesis

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Abstract

R Coronae Borealis (RCB) stars are rare hydrogen-deficient carbon-rich variable supergiants thought to be the result of dynamically unstable white dwarf mergers. We attempt to model RCB stars through all the relevant timescales by simulating a merger event in Octo-tiger, a 3D adaptive mesh refinement (AMR) hydrodynamics code, and mapping the post-merger object into MESA, a 1D stellar evolution code. We then post-process the nucleosynthesis on a much larger nuclear reaction network to study the enhancement of $s$-process elements. We present models that match observations or previous studies in most surface abundances, isotopic ratios, early evolution, and lifetimes. We also observe similar mixing behavior to previous modeling attempts that result in the partial He-burning products visible on the surface in observations. However, we do note that our subsolar models lack any enhancement in $s$-process elements, which we attribute to a lack of hydrogen in the envelope. We also find that the $^{16}\text{O}/^{18}\text{O}$ isotopic ratio is very sensitive to initial hydrogen abundance and increases outside of the acceptable range with a hydrogen mass fraction greater than $10^{-4}$.

Unified Astronomy Thesaurus concepts: Close binary stars (254); Stellar mergers (2157); Stellar evolutionary models (2046); Stellar nucleosynthesis (1616); Hydrodynamics (1963); White dwarf stars (1799); R Coronae Borealis variable stars (1327); Abundance ratios (11)

1. Introduction

R Coronae Borealis (RCB) stars are rare hydrogen-deficient, carbon-rich supergiants (Clayton 2012, 1996). They are best known for their irregular variability of up to 8 mag induced by dust formation in their atmospheres. RCB stars are suspected to be a result of a binary white dwarf (WD) merger event consisting of a carbon–oxygen (CO) and a helium (He) WD (Webbink 1984). The surface abundances of RCB stars not only are extremely helium rich and hydrogen deficient but also contain an enrichment in N, Al, Na, Si, S, Ni, and several $s$-process elements (Asplund et al. 2000). Furthermore, RCB stars show extraordinarily low $^{16}\text{O}/^{18}\text{O}$ (on the order of unity) and large $^{12}\text{C}/^{13}\text{C}$, which, along with the enrichment of $s$-process elements, are consistent with partial He burning (Clayton et al. 2007). The mass ratio of the WD merger should be between 0.5 and 0.6, with the total mass ranging between 0.7 and 1.0$M_\odot$ based on the requirement of dynamically unstable mass transfer (Dan et al. 2011; Zhang et al. 2014) and the high-temperature region required for partial He burning (Staff et al. 2012).

Previous attempts to model RCB stars utilize “stellar engineering” (described in Section 2.1; Lauer et al. 2019; Crawford et al. 2020), modified evolution of zero-age main-sequence stars (Weiss 1987; Menon et al. 2013, 2019), and mapping of 3D merger simulations into a 1D stellar evolution program (Schwab 2019). Of those methods, the first two attempts to mimic the thermal properties of the post-merger object based on hydrodynamics simulations. This work attempts to model RCB stars with the third method, which directly takes into account the thermal structure from the 3D merger model resulting from the dynamical merger.

In this paper, we construct the binary system in a 3D adaptive mesh refinement (AMR) hydrodynamics code called Octo-tiger (Marcello et al. 2016). After the merger event, we perform a volume weighted spherical average of the evolved parameters. Using Modules for Experiments in Stellar Astrophysics (MESA) version r12115 (Paxton et al. 2011, 2013, 2015, 2018, 2019), we implement the built-in relaxation algorithms to construct a 1D model of the post-merger object and let it evolve through the RCB phase and back down the WD cooling track. Once the stellar evolution calculations are finished, the model is then post-processed with a more complete nuclear network using the NuGrid multizone nucleosynthesis code MPPNP (Herwig et al. 2008). This post-processing analysis of the nucleosynthesis happens for every zone at every time step of the stellar evolution and includes 1093 isotopes with their corresponding nuclear reactions.

The models presented in this paper make improvements on what has been done in previous models using smooth particle hydrodynamics (SPH) codes or “stellar engineering” in MESA (Dan et al. 2011; Longland et al. 2011; Staff et al. 2012; Menon et al. 2013; Zhang et al. 2014; Staff et al. 2018; Menon et al. 2019; Lauer et al. 2019; Schwab 2019; Crawford et al. 2020). In the following sections we compare our initialization process to other works that simulate RCB stars (Section 2), present our numerical methods in generating these models (Section 3), present the results of our parameter studies on our models (Section 4), and follow up with concluding thoughts on improvements we will make to these models (Section 5).

2. Comparison with Previous Work

In this section, we describe how our models are initialized differently than previous studies. In particular, we focus on the thermal structure, the nuclear network, and the mechanisms for chemical mixing.
2.1. Initialization of Thermal Structure

In general, there have been three methods used to generate the thermal structure of an RCB star. Those methods are the He star model, stellar engineering, and mapping a spherically averaged structure from a 3D hydrodynamics code.

The He star model is employed in works such as Weiss (1987) and Menon et al. (2013, 2019). This model is initialized with a helium zero-age main-sequence star, and after the envelope has shrunk to some predetermined mass, a composition motivated from realistic progenitor models is imposed on the envelope. Menon et al. (2013) split the abundance profile into four zones that are initialized based on progenitor models. Those zones are the core, a buffer region to prevent dredge-up from the core, the He-burning region, and the envelope. The separate initialization of the He-burning region based on nuclear burning during the dynamical phase is a more sophisticated approach that is not considered in our models. This provides a CO core consistent with core He burning underneath an He-burning shell and an envelope with the expected composition. However, the thermal state of the core is not in agreement with what would be realized in a WD merger scenario, and this will have effects on the evolution and state of the envelope (Iben 1990; further discussed in Section 4.1.1). In the WD merger scenario, one should expect the CO WD that would form the core of the RCB to be cooler and more degenerate than the CO core that would form from core He burning. The additional entropy taken into account at the core–envelope boundary from the dynamical merger event leads to convective mixing in the envelope. Menon et al. (2013) do not see a convective envelope and instead require a secular mixing model be adopted to account for the required envelope mixing and justify that the additional mixing may be induced by rotation.

Stellar engineering is a general term used to describe any ad hoc change to the numerical model that is not implemented through a physical process in order to construct a stellar model that matches some expected initial structure. One way to use stellar engineering to create RCB stars is discussed in great detail in Lauer et al. (2019) and Crawford et al. (2020). This process provides a more physically motivated structure than the He star method, as it creates a cool and degenerate CO core. In order to get He shell burning and the desired post-merger radius, a process of adjusting the entropy as described in Shen et al. (2012) is employed to add entropy to the envelope until the desired post-merger radius of 0.1R⊙ is reached. This method also generates enough mixing via convection to bring species from the He-burning region to the surface.

Mapping data from a 3D hydrodynamics code is the method used in this paper, as well as studies such as Longland et al. (2011) and Schwab (2019). Schwab et al. (2012) took 3D models from Dan et al. (2011) and performed 2D simulations of the viscous phase of the merger with α-viscosity prescription. Those models evolve into spherical states on the order of a few hours and are then mapped into the 1D MESA grid and explored further in Schwab (2019). Our models do not contain a prescription for viscosity and therefore will not naturally evolve into spherical states. Furthermore, there is difficulty when mapping the thermal structure because of any mismatch in the equation of state (EOS) between two different codes. Like Schwab (2019), our models use the Helmholtz EOS to compute the temperature, which assumes full ionization, and therefore the Helmholtz EOS and MESA should match well near the peak temperature region. There is, however, a discrepancy due to the fact that MESA assumes that the object is in hydrostatic equilibrium (HSE), which is not the case for the post-merger object coming out of Octo-tiger. More details regarding this discrepancy can be found in Section 3.2.

2.2. Nucleosynthesis and Mixing

When comparing surface abundances in constructed models to observations, it is important to consider key isotopes and reactions, as well as mixing. Most studies include at least a basic nuclear network using H, He, C, N, O, and F, but for investigating s-process nucleosynthesis it is also important to include neutron-source and neutron-capture reactions, as well as more massive species. In our models we use the MESA nuclear network mesa.75.net (herein referred to as mesa_75) for co-processing, as it includes neutrons and species up to 66Zn. Post-processing is then done with 1093 species in MPPNP, and because of our large co-processed network, our models are usually consistent for the most prominent species. The MESA calculated convective regions are used to inform mixing in the post-processing stage as well. While some of the below studies have considered the effects of rotation-driven mixing, we do not utilize those mixing prescriptions because convective mixing was sufficient in bringing the partial He-burning products to the surface.

Lauer et al. (2019) used mesa_75 for co-processing as well, but they do not perform any post-processing. However, they see good agreement with 16O/18O and C/O, as well as surface abundances during the RCB phase. In terms of mixing, both convection and rotationally induced mixing are used in order to transport the species from the burning region to the surface. However, only solar metallicities are considered in their study, but the observations of most RCB stars show subsolar metallicities (Asplund et al. 2000; Clayton et al. 2007). Crawford et al. (2020) expand on those models by analyzing models with subsolar metallicities using the same stellar engineering method.

Menon et al. (2013, 2019) study solar and subsolar metallicities, respectively. These studies take extra care to analyze the nucleosynthesis responsible for the overabundance in 18O and 19F. They find that they are only able to reproduce the surface abundances with a particular mixing profile that mixes material not so fast as to destroy all of the 18O but fast enough to bring 15N to the burning region in order to form 19F. This mixing profile is implemented by creating an additional diffusion coefficient that is justified to be the result of rotationally induced mixing. Furthermore, this additional diffusion coefficient must halt before the RCB phase in order to maintain the surface 14N abundance. Their study also uses post-processing with over 1000 isotopes and investigates s-process elements but finds that only lower mass ratios (q = 0.5) have a neutron number density high enough to produce s-process elements.

Zhang et al. (2014) build a custom nuclear network within MESA containing 35 species up to 32S and 113 reactions. However, this network does not include neutrons and thus cannot produce s-process elements. As is the case in our study and other studies, mixing via the mixing-length theory (MLT) prescription in MESA is sufficient to bring species from the burning region to the surface (Lauer et al. 2019; Crawford et al. 2020).

Schwab (2019) chooses not to focus on the nucleosynthesis given the limitations of the nuclear network used in
Schwab et al. (2012). However, he does emphasize the importance of a modified opacity table, as the default opacity tables used in MESA are not well suited for following the evolutionary tracks of RCB stars. The default opacity table in MESA is calculated using GS98 (Grevesse & Sauval 1998) solar-scaled abundances. Although MESA does include opacity tables used in MESA are not well suited for following the evolutionary tracks of RCB stars. The default opacity tables and do not explore this parameter further.

### 3. Methods

Our post-merger simulations build on previous work done using “stellar engineering” in MESA (Lauer et al. 2019). In the previous approach, a post-merger structure was constructed in order to mimic a thermal and chemical structure consistent with that found in past 3D hydrodynamics merger simulations. The effects of rotation were included by assuming solid-body rotation with 20% breakup velocity. Then, the post-merger evolution is followed to the RCB phase using the MESA 75-isotope nuclear network, mesa_75. The surface abundances, the surface rotation rates, and the time spent in different phases were computed for several models with differing mass parameters.

The work presented here uses one 3D hydrodynamics model that has either a solar- or subsolar-metallicity composition imposed onto the post-merger object. In each choice of metallicity, the evolution of the post-merger object is followed through the RCB phase and back to the WD state. The initial conditions and results of each model are summarized in Table 1. The following subsections outline the procedure used to map the 3D hydrodynamics grid into MESA and process the RCB data.

#### 3.1. Progenitor Evolution

The first step in RCB evolution is a CO+He WD merger event. In order to form a single star, there are two important requirements for the close binary WD (Zhang et al. 2014). First, the mass parameters and the initial separation must be such that the system loses angular momentum and causes the separation to decay until the He WD fills its Roche lobe. Second, once the He WD begins to lose mass, its radius will increase more rapidly than the separation due to the transfer of angular momentum. These two requirements will lead to a
dynamically unstable merger event and constrain the mass ratio between 2/3 and 1. However, there are situations in which the spin–orbit coupling results in a dynamically unstable merger event while having a mass ratio less than 2/3 (Dan et al. 2011). These constraints are illustrated in Figure 1 of Zhang et al. (2014).

Since the surface abundances of RCB stars are consistent with partial He burning, it is important to have a hot shell above the CO core that has a sufficient temperature to ignite He burning. Staff et al. (2012) investigate the effects of the binary mass ratio on He-burning shell temperature and find that the temperature decreases as the mass ratio increases. Of course, the He-burning temperature will also increase as the total mass of the system increases. The necessity for an He-burning shell and an unstable dynamical merger constrains the total mass and mass ratio to 0.7–1.0$M_\odot$ and 0.5–0.7, respectively.

Our 3D hydrodynamics simulation, Octo-tiger, is initialized with a 0.53$M_\odot$ CO WD and a 0.32$M_\odot$ He WD. Octo-tiger uses a simple zero-temperature WD (ZTWD) and ideal gas EOS. The ZTWD EOS assumes a zero-temperature electron gas with a mean molecular weight per free electron of 2 atomic units. The mean molecular weight for ions and electrons used in the ideal gas EOS is calculated for fully ionized He for the primary (4/3 atomic units) and an equal mixture of fully ionized C and O by mass for the primary (1.75 atomic units). The pressure and energy equations used for the ZTWD EOS are shown in Benz et al. (1990) and are shown below in a slightly different form:

\[ P_{\text{deg}} = A[(x(2x^2 - 3)(x^2 + 1)^{3/2} + 3 \sinh^{-1}x)] \]  
\[ E_{\text{deg}} = A[8x^3((x^2 + 1)^{3/2} - 1) - (x(2x^2 - 3)(x^2 + 1)^{3/2} + 3 \sinh^{-1}x)] \]

where

\[ x = \left( \frac{\rho}{B} \right)^{1/3} \]

\[ A = \frac{\pi m_p c^5}{3h^3} \]

\[ B = \frac{8\pi m_p\mu_e}{3} \left( \frac{m_p c^3}{h} \right)^3. \]

While the primary and secondary stars are tracked as fluids, Octo-tiger does not trace abundances, and therefore we cannot directly obtain a composition profile from this simulation. More details of the composition are discussed in Section 3.2. The initial orbital period of the binary is 149 s, and the initial grid is 24,000 subgrids with up to seven levels of refinement. The refinement criterion is based solely on the density. Because Octo-tiger does not handle gravitational radiation or magnetic fields, angular momentum is removed from the system at a user-defined rate. For this system, the dynamically unstable merger event initiates after about an hour. After 3.3 hr of evolution in Octo-tiger, we spherically average the grid to be mapped into MESA. Equatorial and polar slices of the density and temperature are shown in Figures 1, 2, 3, and 4. In Figures 3 and 4, a hot shell is clearly visible and has a peak temperature of about 285 MK, which is notably lower than the models in Lauer et al. (2019), but still high enough to initiate He burning as seen in Figure 5.

In order to compute the spherically averaged parameters, the following procedure was implemented. First, the center of mass was found by finding the 3D grid cell with maximum density, and then all positions are translated so that the center of mass is at the origin. Next, we create roughly 350 spherical shells centered on the origin with radius $r$ and thickness $dr$ such that $\log_{10} r$ is constant. This binning in log-space and resolution helps to ensure that we get good resolution near the He-burning region and in the outer layers of the star. For each shell, we sum the product of a parameter $X_r$ and cell volume $dV_r$ for all cells in between a radius $r$ and $r + dr$ and divide by the volume of the shell to get the spherically averaged parameter $X_r$ at radius $r$ (shown in Equation (5)). Additionally, we compute the total energy of each shell as the sum of the spherically averaged bulk kinetic energy and a calculated potential energy (Equation (6)). The radius of the spherical post-merger object is then taken to be the outer radius where the material is bound. For this system, we obtain a radius of 0.50$R_\odot$ and a total bound mass of...
Mapping into the Spherical Grid of MESA

The second step of the RCB simulation is the nuclear timescale evolution from the post-merger object through the RCB phase back to a WD state. This evolution is done by mapping our spherically averaged post-merger object into MESA using the MESA built-in relaxation algorithms. A discussion of how MESA relaxes models can be found in Section B of the Appendix in Paxton et al. (2018). In order to map this object into MESA, three profiles are required: composition, specific angular momentum, and entropy. Assumptions and methods used to obtain those profiles are outlined in the remainder of this subsection.

Assuming that both components of the post-merger object are well mixed, we impose two different uniform compositions for the CO and He WD. The composition is obtained by running the MESA test suite problems make_co_wd and make_he_wd for the solar and subsolar metallicities. The metallicity fractions used in these models were the MESA default options from Grevesse & Sauval (1998). We then impose the CO WD composition on the post-merger object up to the mass coordinate corresponding to the original mass of the CO WD (0.53\(M_\odot\) in our system). Next, we impose the He WD composition from the mass coordinate of CO WD onto the surface. An illustration of this composition can be found for some key elements in Figure 6. This assumes that any mass lost in the system is only lost by the He WD, which is a good assumption since the He WD experienced a tidal disruption while the CO WD remained mostly inert and intact. Because Octo-tiger does track the components as fluids, one could in principle use the component fractions in each cell to calculate an abundance assuming that the WDs were well mixed and had a homogeneous composition. However, these AMR simulations tend to overestimate the amount of material dredged up from the primary compared to other hydro simulations (Staff et al. 2012, 2018). Staff et al. (2018) claim that mixing during the dynamical merger phase has important effects on the surface abundance. In particular, it is important to avoid dredging up too much material from the primary, as it could create an overabundance of \(^{16}\text{O}\) and make it difficult to produce a sufficient amount of \(^{18}\text{O}\) in order to obtain the isotopic ratio of order unity. Therefore, we find the method of imposing a composition based on mass coordinate to be more reliable.

The angular momentum comes directly from the 3D hydrodynamics grid by computing the axially symmetric angular momentum from the linear momentum and the radius as seen in Equation (7). After computing the specific angular momentum for each cell, it is averaged using Equation (5) with clearly not spherical in Figure 2. However, Schwab et al. (2012) find that these systems tend toward spherical states on the timescale of a few hours. We attribute the toroidal shape of our system to the fact that Octo-tiger does not have a prescription for viscosity and thus, other than numerical diffusion, there is no physical mechanism to diffuse angular momentum. We find that spherically averaging this system reduces the He-burning region temperature by a factor of two, which is likely due to the nonspherical state of the system “smearing” the peak temperature over the polar angle. It is important to note here that, due to the high sensitivity that nuclear reactions have on temperature, these small factors could result in large changes in composition during post-merger evolution.

### 3.2. Mapping into the Spherical Grid of MESA

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The immediate problem with obtaining the entropy profile from Octo-tiger is that the entropy is not an evolved variable and uses a much simpler EOS than MESA. The ZTWD and ideal gas EOS of Octo-tiger will not match the EOS tables used by MESA, especially in extreme regions of high density and high temperature. Figure 50 of Paxton et al. (2019) shows the density–temperature coverage of the EOS used in MESA. Rather than directly relax an entropy profile, MESA can compute an entropy profile by relaxing a density and temperature profile. This is the method we implement because it allows us to compare density and temperature profiles to the previous work in Lauer et al. (2019), and we can produce an informed temperature structure of the CO core. The density profile is simply spherically averaged from Octo-tiger, but the temperature profile needs to be computed using the evolved internal energy density. Using the Octo-tiger internal energy density and the composition profile we imposed on the post-merger object, we compute a temperature profile using the Helmholtz EOS (Timmes & Swesty 2000). Because Octo-tiger assumes a ZTWD EOS in the highly dense CO core, we floor this temperature to a constant value of 10 MK. The density and temperature profiles are then combined for relaxation in MESA.

After computing the necessary three profiles, the MESA relaxation routine is implemented. Figure 5 shows some of the profiles of the spherically averaged Octo-tiger output and the relaxed MESA model for comparison. Figure 5 also shows a density–temperature profile for the Octo-tiger output and the MESA relaxed model with the He-burning and C-burning regions illustrated. Of these profiles, the only parameter that has a significant difference between the Octo-tiger value and MESA relaxed value is the temperature (in which the peak relaxed temperature is a factor of 1.5 higher than the peak Octo-tiger temperature). We attribute this to the conversion of the Octo-tiger internal energy not being hydrodynamically stable with the density profile in MESA. However, the peak temperature is still high enough to commence He burning, a necessary ingredient to obtain the surface abundances observed in RCB stars. It should, however, be noted that even a small range of peak temperature values may significantly change the

\[ j = r \times p = x p_{y} - y p_{z}. \]  

\[ \text{Density} \ [g/cm^3] \]

\[ \text{Temperature} \ [K] \]

\[ \text{Specific Angular Momentum} \ [m^2/s] \]

\[ \text{Density} \ [g/cm^3] \]

\[ \text{Temperature} \ [K] \]

\[ \text{Mass Fraction} \]

\[ q \] is the normalized exterior mass coordinate \((q = 1 - \frac{M}{M_{\text{tot}}})\).

Figure 5. Comparison of the spherically averaged final Octo-tiger output (dashed) to the MESA relaxed output (solid). \( q \) is the normalized exterior mass coordinate \((q = 1 - \frac{M}{M_{\text{tot}}})\).

Figure 6. Abundance profiles for key species in Model 1 from Table 1. The effects of nuclear burning in the hot He shell (or SOF) that has taken place up to that phase can be seen around \( q \sim 0.7–0.8 \).

\[ \text{http://cococubed.asu.edu/code_pages/eos.shtml} \]
outcome of the surface abundances during the RCB phase. Crawford et al. (2020) analyze the effect of peak temperature on surface abundance during the RCB phase.

3.3. Nucleosynthesis Post-processing

The last step in the RCB simulation is to post-process the data with a much larger scale nuclear network using the NuGrid MPPNP code (Herwig et al. 2008). Since MPPNP is a post-processing code, it does not change the evolution of the star, but it performs nucleosynthesis calculations for all isotopes— including those involved in the s-process. This builds in the assumption that the energy produced from the high-mass nucleosynthesis does not contribute to the stellar structure and the mesa_75 nuclear network accounts for almost all of the nuclear energy generation. The post-processing code also mixes the species after each time step in accordance with the MESA simulation.

After evolving the post-merger object, we take the stellar profile at the point where the surface temperature is at a minimum and luminosity is at a maximum; this is how we define the RCB phase. At this phase we calculate the surface abundances, as well as isotopic ratios of interest for RCB stars. Table 1 contains the isotopic ratios, and Figure 7 contains the surface abundances at the RCB phase for the best-matched models. The surface abundances are calculated using the typical Equation (8). In this equation, $X$ is the average mass fraction of an element of all zones with optical depth less than 1, $\mu_X$ is the mean atomic mass of that element, and $\log \epsilon(X)_\odot$ is the solar value of that element taken from Lodders (2003). This value represents the log of the number of ions of element $X$ in a sample containing $10^{12.15}$ ions normalized to the solar value:

$$[X] = \log X - \log \mu_X + 12.15 - \log \epsilon(X)_\odot. \quad (8)$$

4. Results

In this section, we discuss the results from our evolutionary models. We start by discussing our initial models for solar and subsolar metallicities. Next, we discuss variations of those cases as we implement varying degrees of overshooting and change the initial abundance of hydrogen in the RCB envelope.
Finally, we use the models that best match observations from the solar and subsolar cases and post-process them with the NuGrid MPPNP code for analysis of s-process elements.

4.1. Initial 3D to 1D MESA Models

In this section we discuss the results from our base solar and subsolar models that contain no overshooting and no initial hydrogen adjustment (Model 1 and Model 22) for comparison against the engineered models of Lauer et al. (2019). Specifically, we focus on the early stages of evolution following the merger and the mixing that takes place. Then, we discuss how changes in overshooting or initial hydrogen abundance affect the results.

4.1.1. Early Stage Evolution

The primary goal of this study is to obtain results similar to observations and compare to those obtained by the stellar engineering procedure of Lauer et al. (2019). In their study, they explore a parameter space consisting of initial radius, total mass, mass ratio, rotation, and initial hydrogen abundance. Of those initial parameters, their model A7 is most similar to our initial conditions in terms of total mass, mass ratio, and initial hydrogen ratio. The major differences in our model are that the initial rotational profile, thermal profile, and radius of the post-merger object are calculated based on the Octo-tiger grid. After mapping the 3D merger object from Octo-tiger into MESA using the procedure outlined in Section 3, we let it evolve and obtain an HRD track shown in Figure 8.

The HRD tracks in this study are similar to those of Lauer et al. (2019) and Schwab (2019), with an early brightening phase leading the model into the RCB box (the observed range of effective temperatures and luminosities of RCB stars) from the bottom. This is different from the models of Weiss (1987) and Menon et al. (2013, 2019), which see a small brightening and cooling phase preceding the models to enter the box from the left. This is the result of the 3D merger and engineered models starting off with more compact and cooler cores. The envelope then expands as a result of the energy released from the steady He-burning shell. There is a short period of thermal adjustment in the envelope as the He-burning shell reaches a steady state, after which the solar and subsolar models have identical tracks in the HRD. This thermal adjustment lasts around 500 yr and expands the envelope until log$(L/L_\odot)$ reaches 2.5–2.7. Schwab (2019) also sees this thermal readjustment phase in his multidimensional model (ZP4) mapped into MESA with similar lifetimes (though that model starts off much brighter than ours). The time it takes for the solar and subsolar models to enter the RCB phase (minimum effective temperature) is 1600 and 1300 yr, respectively. This is in agreement with the lifetimes reported in Lauer et al. (2019) and the higher He-burning temperature models of Crawford et al. (2020).

4.1.2. Surface Abundance and Mixing

While Lauer et al. (2019) do not report surface abundances from model A7, they do report surface $^{16}$O/$^{18}$O of about 35 and C/O of about 4.6. This differs from our values of 3.05 and 75.56 significantly. Our $^{16}$O/$^{18}$O ratio is in better agreement with observations (Clayton et al. 2007), but our C/O is significantly higher than the observed values (∼1). The reason for this is predominantly due to the difference in early evolution. In our models, the temperature profile of the He envelope evolves rapidly during the thermal adjustment phase, causing differences in the early mixing of elements by convection and the peak temperature getting as high as 400 MK for a brief time, which is illustrated in Figure 9. Within the first year of evolution, two distinct convective regions form in the He envelope of the star separated by a temperature inversion. The inner convective region reaches from the He-burning region to the temperature inversion, and the outer region reaches from the top of the temperature inversion to the surface. This temperature inversion appears to evolve from bumps in the temperature profile, which are likely caused by the initial spiral structure of the merger seen in Figure 3. This temperature inversion is present and evolves similarly across all
models in this study. We also note that because this first convection gap is eventually bridged in all of our models, its importance to the surface abundance during the RCB phase is minimal. Lauer et al. (2019) and Schwab (2019) show temperature–density profile plots for engineered models that are much smoother and do not have this temperature inversion present. However, Schwab (2019) does not focus on nucleosynthesis, and hence mixing is not as important in his study, and Lauer et al. (2019) do not perform a detailed analysis of their mixing profile.

A clearer presentation of how this affects the mixing is shown in Figure 10. The first convective gap caused by the spiral structure can be seen around 0.77$M_\odot$ for the first 40–50 yr of evolution. Furthermore, we note that the mixing region between the surface and He-burning shell becomes disconnected after about 30 yr, which explains why we see evidence of partial He burning in RCB stars. The second convective gap is also a feature of the stellar engineered models of Crawford et al. (2020). Because this second convective gap disconnects the surface from the burning region, the surface abundances become set and remain static after that point. This means that the surface abundances are solely dependent on the burning that happens in the first 30 yr in our models.

4.1.3. Robustness of Convective Solution

Convection is an important feature that brings the partially synthesized material from the burning region to the surface. In order to ensure that convection is a robust feature in our models, we made three test cases with different initial conditions in order to test whether or not convection persists in the envelope. Two of these test cases use a different averaging procedure described in Endal & Sofia (1976), which averages cells on equipotentials (including the effects of rotation) instead of radial shells. One of the equipotential-averaged models uses mass weights during the averaging procedure (replacing $d\rho$ with $dm$ in Equation (5)), and the other uses volume weights. The third model uses the density profile obtained by the equipotential averaging procedure with volume weights in order to find a temperature profile in HSE. This is done by using the equation for HSE (Equation (9), where $\Psi$ is the effective potential) and the calculated density profile in order to calculate a pressure profile:

$$\frac{dP}{dr} = -\rho \nabla \Psi.$$

Then, we use the Helmholtz EOS to calculate temperature given pressure and density and apply the same procedure outlined in Section 3 in order to insert the degenerate CO core. Figures 11 and 12 show the profiles of Model 1 and the HSE model at key phases during their evolution, respectively.

The temperature-density profiles of these three models and Model 1 are illustrated in Figure 13 for direct comparison. The purpose of these models is simply to demonstrate that the convective instability persists in the envelope independent of the initial averaging procedure we used. Therefore, it is important to note here that these test models are simplistic in terms of the nuclear network and initial composition. The nucleosynthesis in these models may be unreliable, and we therefore choose not to analyze the surface abundances during the RCB phase.

These test cases show that despite starting with a different averaging procedure and therefore a different initial thermal profile, these models converge to similar solutions on the order of 10–100 yr. All three test models show the same behavior of two distinct convective regions separated by an initial convective gap that eventually merge and a second convective gap forming around the same time, causing only partially synthesized material to mix at the surface of the star. We illustrate this in Figures 11 and 12 for Model 1 and the HSE test model, respectively. In the top panels, we see the initial convective (left) and temperature (right) profiles, as well as the initial composition (labeled in the legend). The middle panels show the profiles right after two distinct convective regions form, separated by the temperature inversion discussed in Section 4.1.2. The bottom panels show the moment right after the convective gap closes and synthesized material is allowed to mix to the surface. At this time, the convective region has already receded from the burning region as the star expands, and material at the surface will not be synthesized further. This behavior is observed in all of our models regardless of the averaging procedure and demonstrates the robustness of our convective solution. There are, however, fairly large differences in the age of the star at which the first convective gap closes (bottom panel), which would result in differences in nucleosynthesis and therefore surface abundances. This is something we aim to explore in more detail in future studies.

4.2. Overshooting

In this study, we vary the strength of overshooting and analyze its effects on the surface composition. MESA version r12115 contains many parameters for overshooting that change the depth into the convective region (overshoot_f0) and the decay length scale outside of the convective region (overshoot_f) in fractional pressure scale heights. For both overshooting options, there are 12 parameters associated with different regions of the star (nonburning core, nonburning shell (above and below), H-burning core, H-burning shell (above and below), etc.). In this study, we vary all overshoot_f parameters and maintain a constant overshoot_f0 parameter of 0.004. Previous RCB studies have not considered overshooting, but it is an expected physical phenomenon that should be included as one considers more physically motivated models. We maintain overshooting parameters within a
reasonable range as discussed in Stancliffe et al. (2015). The results of this study can be found in Figures 14 and 15, as well as Table 1.

In these results, we see a monotonic decrease in the surface abundance of N with increasing overshooting parameter as seen in Figure 15. Crawford et al. (2020) varied the He-burning shell temperature and observe a decreasing N abundance with an increasing He-burning region temperature. In both cases, $^{14}N(\alpha, \gamma)^{16}F(\beta^+)^{18}O$ is being enhanced, thus decreasing the amount of N at the surface. This is consistent with the increase in O seen in Figure 15, while $^{16}O/^{18}O$ remains constant up to an overshooting parameter of 0.07, meaning that there is an enhancement in the production of $^{18}O$ at the same rate as $^{16}O$. Beyond an overshooting parameter of 0.07, $^{16}O$ is dramatically
enhanced by mixing from the CO core. The $^{14}$N($\alpha, \gamma$)$^{18}$F($\beta^+$)$^{18}$O reaction is paramount in the creation of $^{18}$O at the levels seen in observations and is discussed in great detail by Clayton et al. (2007) and Menon et al. (2013). Lastly, as the overshooting parameter increases, we also see a slight increase in Ne. This happens as $^{18}$O undergoes $\alpha$-capture and $^{22}$Ne is created, thus increasing $^{16}$O/$^{18}$O even more. Crawford et al. (2020) also note these key reactions and show that the sum of N, $^{16}$O, and Ne is effectively constant as a function of He-burning temperature. This indicates that these isotopes are almost exclusively affected by just the $^{14}$N($\alpha, \gamma$)$^{18}$F($\beta^+$)$^{18}$O($\alpha, \gamma$)$^{22}$Ne reaction chain.

In this study, we cannot change the He-burning temperature of different models, due to the fact that it is self-consistently calculated within the 3D hydrodynamics merger simulation. However, by introducing stronger amounts of overshooting, we are more efficiently bridging the second mixing gap seen in Figure 10. This allows more time for isotopes to synthesize in the He-burning region and mix to the surface before the convective region breaks from the stellar surface. As the strength of overshooting increases beyond an overshoot$_f$ value of 0.1, the overshooting beneath the He-burning shell begins to bring up material from the CO core at an overwhelming rate. Since the primary isotopes in the core are $^{12}$C and $^{16}$O at a 1:2 ratio, $^{16}$O/$^{18}$O increases dramatically while C/O decreases to the order of unity.

The same study is done with subsolar models for a subset of the overshooting parameters in this study. The results are shown in Table 1, Models 26–30, and we see similar results in the trend of C/O and $^{16}$O/$^{18}$O.

4.3. Initial Hydrogen Abundance

Zhang et al. (2014) point out the important role of the thin hydrogen envelope in the He WD phase. They point out that if more of this hydrogen envelope were to survive, more $^3$He would also survive. In our models, however, there is also a significant abundance of $^7$Li that survives in the thin hydrogen envelope, which later affects the surface abundances during the RCB phase.

Because we mass average the entire He WD, these abundances in the thin hydrogen envelope have a noticeable effect on the initial uniform abundance of the post-merger He envelope. This is especially true for light elements that are otherwise uncommon in the He WD ($^4$He, $^3$He, and $^7$Li, specifically). In order to study the effects of this process, we vary the initial hydrogen abundance in the He envelope while maintaining an overshoot$_f$ value of 0. The results are shown in Figures 16 and 17. There are studies such as Staff et al. (2012) that show a relationship between He WD mass and the mass of the thin hydrogen envelope and would then set the mass fraction of hydrogen in the envelope of the RCB progenitor. However, we justify varying the initial hydrogen mass fraction because any hydrogen burning during the dynamical merger phase is not included in our simulations since Octo-tiger does not include nucleosynthesis. By varying this parameter, we are analyzing the effects of more hydrogen burning during the dynamical phase of the merger, assuming that the energy generation does not significantly alter the structure of the star.

As expected, the surface abundance of $^7$Li goes down with an increasing hydrogen abundance via $^7$Li($\alpha, \gamma$)$^8$Be. Also, there is a large increase in $^{18}$O accompanied by a significant decrease in $^{16}$O between the models with initial H mass fractions of $10^{-4}$ and $10^{-3}$. The decrease in $^{18}$O can be attributed to the enhancement of proton-capture reactions on both $^{16}$O (slightly starving the $\alpha$-capture reaction) and $^{18}$O. The increase in $^{18}$O is also due to the enhancement of the proton-capture rate on $^{16}$N. This is clear by the enhancement in $^{16}$N in the burning region of the higher hydrogen abundance model, which indicates that $^{14}$N($p, \gamma$)$^{15}$O($\beta^+$)$^{15}$N is active. From there, the CNO cycle can branch into $^{15}$N($p, \gamma$)$^{16}$O or $^{15}$N($p, \gamma$)$^{16}$C (which can then $\alpha$-capture or start another CNO cycle). The increase in $^{16}$O and the decrease in $^{18}$O explain the sudden decrease in $^{22}$Ne, seen in Figure 17, as they starve the $^{14}$N($\alpha, \gamma$)$^{18}$F($\beta^+$)$^{18}$O($\alpha, \gamma$)$^{22}$Ne reaction chain of the initial $^{14}$N $\alpha$-capture.

4.4. NuGrid Post-processing

The final section of this study discusses post-processed nucleosynthesis on a much larger nuclear network containing 1093 isotopes and over 14,000 reactions. We chose two models,
one with solar metallicity and one with subsolar metallicity, that are most consistent with previous stellar engineering attempts and observations (Models 17 and 31, respectively). Figure 7 shows the results of these models and the MPPNP post-processed results. Below we explain some of the differences between the MESA and MPPNP models, including surface Li, N, and s-process elements.

4.4.1. Lithium

The biggest difference between MPPNP and MESA surface abundances in Figure 7 is the surface abundance of $^7$Li. This is observed in both the solar and subsolar models. MPPNP burns about 6 orders of magnitude more $^7$Li because it includes the $^7$Li($\alpha$, $\gamma$)$^{11}$B reaction while mesa_75 does not. Typically, $^7$Li would be burned immediately by proton-capture reactions, but in both the solar and subsolar models there is very little initial hydrogen in the He envelope. This low amount of initial hydrogen causes other problems, specifically in the subsolar case, where the initial hydrogen is $10^{-10}$, which is further discussed in Section 4.4.3.

It is important to note that in MESA version r12115 the default $^7$Li($\alpha$, $\gamma$)$^4$He reaction has a sudden cutoff at a temperature of 10 MK. When simulating the He WD progenitor, this cutoff results in a fairly large amount of $^7$Li in the hydrogen envelope, which produces an unusually high initial abundance in the He envelope of the post-merger. In reality, the $^7$Li should have likely been burned away during the evolution of the He WD or during the tidal disruption phase of the merger event. However, since Octotiger does not perform nucleosynthesis or trace the species from each progenitor, the nuclear burning in the merger phase is not considered.

Given that the post-merger object in MESA is not burning $^7$Li via $\alpha$-capture and the initial $^7$Li abundance should be much lower for the above reasons, we do not expect to see any measurable amount of $^7$Li on the surface of our models. This is demonstrated by the results of the MPPNP post-processing and is in agreement with all but four RCB observations (Jeffery et al. 2011). It is still difficult to explain why $^7$Li is abundant in these four observations given the expectation that it all be burned during the merger process (Clayton et al. 2007). We do not explore the lithium problem any further, as it is outside the scope of this paper.
4.4.2. Nitrogen

The surface N abundances in MPPNP are consistently higher than in MESA, and we attribute this to the burning of $^7\text{Li}$ via $\alpha$-capture. $^{14}\text{N}$ can be created in MPPNP via the $^7\text{Li} (\alpha, \gamma)^{11}\text{B}(\alpha, n)^{14}\text{N}$ reaction chain, while the mesa network does not contain $^{11}\text{B}$. This is consistent with the fact that we see a larger enhancement of $^{14}\text{N}$ in the subsolar case, where there is more $^7\text{Li}$ to be burned.

It is worth mentioning that although all four models have lower surface N abundances than observations, this result is still consistent with the engineered models of Crawford et al. (2020). Their hot models (>320 MK) also show diminished $^{14}\text{N}$ and attribute that to enhanced $\alpha$-capture. Our models reach a maximum temperature around 400 MK during the thermal adjustment of the envelope, which coincides with the time where most of the nucleosynthesis takes place. This decrease in $^{14}\text{N}$ is also associated with a sudden burst of neutrons from the $^{22}\text{Ne}$ source, which becomes active above 250 MK (Käppeler et al. 2011). Following the neutron burst, $^{14}\text{N}$ then acts as a neutron poison and is rapidly burned by neutron capture reactions. Both enhancements in $\alpha$-capture and neutron-capture reactions would then result in the observed enhancements of $^{18}\text{O}$ and $^{19}\text{F}$, respectively. $^{14}\text{N}$ can be replenished to observed levels by adding a higher initial hydrogen abundance to the He envelope, but as seen in Figure 16, this increases the oxygen isotopic ratio beyond the acceptable range.

4.4.3. $s$-process Elements

One characteristic of RCB stars is their enhancement in $s$-process elements on the surface (Jeffery et al. 2011). Previous studies in stellar engineering and our MESA models do not include $s$-process nucleosynthesis, but MPPNP does. Figure 7 shows that the solar case has a slight enhancement of $s$-process elements (Sc, Y, Zr, Ba, and La), but the subsolar case does not see this enhancement. The reason we are not seeing $s$-process enhancement is because in both cases we have very little $^{13}\text{C}$ neutron source, which would be active above a temperature of 100 MK (Käppeler et al. 2011). This is a direct result of having a lower initial hydrogen abundance, as the $^{12}\text{C}$ being brought up from the core cannot proton capture to create $^{13}\text{C}$ via $^{12}\text{C}(p, \gamma)^{13}\text{N}(\beta^\pm)^{13}\text{C}$. With a higher hydrogen abundance, we would expect to see more enhancement of $s$-process elements, but this would also push the oxygen ratio outside the observed range (see Figure 16).

5. Conclusions

This study presents the first attempt to reproduce RCB star surface abundances (including $s$-process elements) starting from a 3D hydrodynamics merger simulation. While this attempt is not complete and negates some potentially important phases of nuclear burning (namely, during the merger process), it establishes a mechanism for bringing models from a 3D merger simulation to a full-scale 1D nucleosynthesis
post-processing network. Our models show strong similarities to the stellar engineering models of Crawford et al. (2020) and Lauer et al. (2019) in terms of evolution, mixing, and most surface abundances. Our models also have difficulties in matching $^{14}$N to observations (similar to Crawford et al. 2020) and generating s-process elements.

Our early-stage evolution strongly resembles those of Lauer et al. (2019), Schwab (2019), and Crawford et al. (2020). This is because the stellar engineering process is informed by 3D hydrodynamics models but does not evolve directly from the results of those models. The differences between those models and the He star model of Weiss (1987) and Menon et al. (2013, 2019) are mostly due to how the initial state of the envelope reacts to the input luminosity of the He-burning shell.

While overshooting was necessary in order to match the isotopic ratios, it is a realistic physical phenomenon expected to occur in stars where convection operates and should be included by default in stellar models. Overshooting was not previously studied in the context of RCB stars, but Stancliffe et al. (2015) use models with parameters in the same range as our overshoot parameters. The parameter space of overshoot parameters could be further constrained by 3D models with realistic mixing procedures, but the adopted MLT prescription in MESA is currently the best we can achieve. We find that overshooting parameters of 0.073 and 0.068 for the solar- and subsolar-metallicity models, respectively, yield reasonable agreement to observations and previous studies in surface composition. Lower values tend to increase C/O outside the acceptable range, while higher values tend to increase $^{18}$O/$^{16}$O and decrease surface N outside the acceptable range. There are, however, many other parameters to study that will change the surface composition.

This study also explores the effects of changing the initial hydrogen abundance. The initial hydrogen abundance may change based on how much of the hydrogen shell of the He WD progenitor survives during the merger process. While studies such as Staff et al. (2012) or Driebe et al. (1998) constrain the mass of the hydrogen envelope to values much higher than our models, we note that Octo-tiger does not perform nucleosynthesis during the dynamical merger phase, which may burn a significant fraction of the initial hydrogen. Of course, with too little initial hydrogen (our subsolar model, for instance) the He-burning shell cannot create a sustainable $^{13}$C neutron source. Additionally, there are common envelope phases before the WD merger that are not simulated in this study but will affect the progenitor composition. The complexities of the complete RCB evolution necessitate a wider parameter space study of the initial post-merger composition. Future studies that pursue the 3D simulation of the merger being mapped into 1D nuclear lifetime evolutionary codes like MESA should include a basic nuclear network that accounts for most pp-chain and CNO cycle elements during the merger phase. Being able to trace and burn isotopes during the merger will give improved compositional profiles to be mapped into a 1D evolution code.

In future work, we plan to continue to use this approach to produce more realistic models of RCB stars. Improvements we plan to make include using a basic nuclear network during the merger phase, including a prescription for angular momentum diffusion in order to naturally spherize the merger, creating a customized RCB nuclear network that includes important species of this study for speedup of the MESA simulations (i.e., we do not need to co-process elements beyond $^{26}$Mg at our burning temperatures), and a more careful consideration of opacities and mass loss during the RCB evolution. This is the first in a long line of improvements to be made in modeling RCB stars more realistically. Our attempts to produce better models also necessitate the inclusion of more detailed physical processes during the merger phase, which we will attempt to address in future studies.

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Software: Octo-tiger (Marcello et al. 2016), MESA-v12115 (Paxton et al. 2011, 2013, 2015, 2018, 2019), MPPNP (Herwig et al. 2008), Python (available from python.org), Matplotlib (Hunter 2007), Numpy (van der Walt et al. 2011).

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