MULTIDIMENSIONAL MODELING OF TYPE I X-RAY BURSTS. II. TWO-DIMENSIONAL CONVECTION IN A MIXED H/He ACCRETOREnvironmental

C. M. Malone 1,2, M. Zingale 2, A. Nonaka 3, A. S. Almgren 3, and J. B. Bell 3

1 Department of Astronomy & Astrophysics, The University of California Santa Cruz, Santa Cruz, CA 95064, USA; malone@ucolick.org
2 Department of Physics & Astronomy, Stony Brook University, Stony Brook, NY 11794-3800, USA
3 Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

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ABSTRACT

Type I X-ray bursts are thermonuclear explosions of accreted material on the surface of neutron stars in low-mass X-ray binaries. Prior to the ignition of a subsonic burning front, runaway burning at the base of the accreted layer drives convection that mixes fuel and heavy-element ashes. In this paper, the second in a series, we explore the behavior of this low Mach number convection in mixed hydrogen/helium layers on the surface of a neutron star using two-dimensional simulations with the Maestro code. Maestro takes advantage of the highly subsonic flow field by filtering dynamically unimportant sound waves while retaining local compressibility effects, such as those due to stratification and energy release from nuclear reactions. In these preliminary calculations, we find that the rp-process approximate network creates a convective region that is split into two layers. While this splitting appears artificial due to the approximations of the network regarding nuclear flow out of the breakout reaction $^{18}\text{Ne}(\alpha, p)^{21}\text{Na}$, these calculations hint at further simplifications and improvements of the burning treatment for use in subsequent calculations in three dimensions for a future paper.

Key words: convection – hydrodynamics – methods: numerical – stars: neutron – X-rays: bursts

Online-only material: color figures

1. INTRODUCTION

An accreting neutron star can only build up a thin ($\sim 10$ m) surface layer of H/He before the immense gravitational acceleration compresses this fuel to the point of ignition. The ensuing thermonuclear runaway is short lived ($10$–$100$ s) but releases an enormous flux of X-rays (total energy $\sim 10^{40}$ erg)—a transient event we detect and classify as a Type I X-ray burst (XRB; see Lewin & Joss 1981; Lewin et al. 1993; Bildsten 2000; Strohmaier & Bildsten 2010; in ’t Zand 2011 for reviews). Once the explosion subsides, the accretion builds up a fresh layer of fuel in a matter of hours to days, and a new outburst occurs. An XRB light curve shows a sharp rise—about an order of magnitude increase during $\sim 1$ s—in the X-ray luminosity, followed by an extended ($\sim 10$ s) decay.

Some ultra-compact systems are thought to accrete pure $^4\text{He}$ (4U 1820-30, for example; Cumming 2003). The most common systems, however, likely accrete a mixture of H/He from an evolved companion star (see, for example, the compilation of bursts in Galloway et al. 2008). Depending on the local accretion rate, the $^4\text{He}$ accreted in these systems may either (1) burn stably to form a pure $^4\text{He}$ layer, which then experiences a thin-shell instability resulting in an outburst, or (2) become unstable itself in the presence of helium resulting in a mixed outburst (Fujimoto et al. 1981; Fushiki & Lamb 1987; Cumming & Bildsten 2000; Bildsten 2000). Mixed bursts typically have longer light curves due to the waiting points in the weak nuclear reactions (see Strohmaier & Bildsten 2010 for an overview).

Mixed H/He XRBs are important sites of explosive hydrogen burning via the rp process (Wallace & Woosley 1981; Schatz et al. 2001; Parikh et al. 2014). The nuclear physics of the rp-process nuclei is a focus of the U.S. Department of Energy proposed Facility for Rare Isotope Beams. Understanding the conditions that exist in XRBs is critical to accurately modeling the nucleosynthesis, which may then alter the light curve.

Furthermore, the subset of XRBs exhibiting so-called Photospheric Radius Expansion burst phenomena—whereby the burst’s luminosity is large enough to lift the photosphere to larger radii (lower effective temperature) before settling back down to the neutron star surface—can yield information about neutron star masses and radii (see, for example, Bhattacharyya et al. 2010; Ozel et al. 2010; Steiner et al. 2010). Most of our theoretical understanding on XRBs comes from one-dimensional studies with stellar evolution codes, assuming spherical symmetry. These one-dimensional calculations are able to roughly reproduce the observed energies, durations, and recurrence timescales for XRBs (Taam 1980; Taam et al. 1993, 1996; Woosley et al. 2004; Fisker et al. 2008). Due to their one-dimensional nature, these simulations can use larger reaction networks than multidimensional studies to predict the nucleosynthetic yields from advanced burning stages, such as the rp process, and explore the nucleosynthesis in detail (Schatz et al. 1999, 2001; Woosley et al. 2004; Fisker et al. 2008; José et al. 2010; Parikh et al. 2013). However, the one-dimensional nature prevents the simulations from directly modeling the convection, and simplified models such as mixing length theory (see, for example, Kippenhahn & Weigert 1992) are needed. Recent multi-dimensional simulations have questioned the validity of mixing length theory and emphasized the role of turbulence (Meakin & Arnett 2007; Arnett et al. 2009). If the convection is not modeled properly, then the wrong temperature/pressure history for a fluid element will be obtained, affecting the nucleosynthesis and light curve.

Simulations of the vertical structure of reacting flow on neutron stars are rare. Several models of detonations (Fryxell & Woosley 1982; Zingale et al. 2001; Simonenko et al. 2012) have been done, but these calculations sample density regimes that are not typical of an XRB. Lin et al. (2006) used a low Mach number algorithm to model pure helium bursts in two dimensions, following the rise in temperature and watching...
the development of convection. Cavecchi et al. (2013) used a simplified hydrodynamic model (the vertical direction was treated as hydrostatic) to model flame propagation across the neutron star on length and timescales appropriate to an XRB, but the numerical technique does not allow for detailed understanding of the dynamics at the front, including mixing and turbulence. It is also important to understand whether the convection can bring ashes up to the photosphere (in ’t Zand & Weinberg 2010; Bhattacharyya et al. 2010), altering our interpretation of the radiation.

In Paper I (Malone et al. 2011), we explored the convective dynamics of a pure helium XRB using our low Mach number simulation code, Maestro. Our results differed from those of Lin et al. (2006) in that we found that a much higher resolution is needed to resolve the He burning peak and to properly capture the convective dynamics. Here, we extend the low Mach number methodology to the case of mixed H/He bursts with an extended network that captures the hydrogen burning. Our ultimate goal in this series of papers is to evolve the convective region to the point where we can see a nonlinear rise in the temperature and to assess how the convection impacts the nucleosynthesis.

2. NUMERICAL METHOD

We use the Maestro algorithm as described in Nonaka et al. (2010). Maestro solves the equations of low Mach number hydrodynamics applicable to hydrostatic (HSE) stellar flows—that is, fluid quantities, e.g., density $\rho(x, t)$, are decomposed into radial background, HSE components, $\rho_0(r, t)$, and perturbational components, $\rho'(x, t)$ that govern the dynamics (see Nonaka et al. 2010, for details). The background pressure, $p_0(r, t)$, governs the thermodynamics and is used in place of the total pressure, $p = p_0 + p'$, everywhere except in the momentum equation—an approximation valid for low Mach number flows up to $O(M^2)$. A key feature of this equation set is that sound waves are filtered from the system, enabling long timescale evolution of highly subsonic flows. This manifests itself through an elliptic constraint on the velocity field that captures the effects of compressibility on a fluid element due to localized heating and stratification. The overall algorithm consists of an advection step, using the piecewise parabolic method; a projection step that enforces the velocity constraint; and reactions, coupled via Strang splitting for second-order accuracy (Almgren et al. 2006). We note, however, that this additional term has little effect in a convective layer, but we include it for completeness.

2.1. Microphysics

We use an approximate network containing 10 species, based on the description of Wallace & Woosley (1981), Appendix C. This network approximates the hot CNO burning, triple-$\alpha$, plus rp-process breakout and burning up through $^{56}$Ni. For details, see the Wallace & Woosley (1981) paper, but below we describe some of the features of the approximate network. We note that our implementation follows that description faithfully, but uses updated ReacLib (Cyburt et al. 2010) rates where they exist; Table 1 lists the particular rates used at some stages in the network, along with the version identifier from ReacLib. The stiff system of ordinary differential equations is integrated using the VODE package (Brown et al. 1989).

Figure 1 shows a schematic of the rp-process network outlined in Wallace & Woosley (1981) and used in this paper. The isotopes labeled in black are those explicitly included in the network, in addition to $^1$H and $^4$He; likewise, black arrows indicate reaction rates explicitly calculated, whereas gray arrows denote approximations. For example, in the HCNO cycle, the sequence of reactions $^{14}$O($\beta^+$) $^{15}$N($p, \gamma$) $^{15}$O is restricted by the slowest rate in the sequence, the $\beta^+$ decay. In the approximate network, $^{14}$O (plus a proton) is converted directly to $^{15}$O at a rate given by the $\beta^+$ decay. The two colored circles in Figure 1 denote locations where the nuclear flow can break out of the HCNO cycle and start up the rp-process path to heavier nuclei. Each of these breakout points differs from the previous method of predicting ($\rho h$)$'$ to edges, averaging ($\rho h$)$_0$ to edges, and then constructing the edge state as ($\rho h$)$_0 +$ ($\rho h$)$_{edge}$. This change is more in line with the original reconstruction described in Almgren et al. (2006), and that used in Zingale et al. (2013), but continues to be a subject of algorithmic investigation.

Additionally, all the models we run here include the additional term in the momentum equation identified by Klein & Pauluis (2012) and Vasil et al. (2013) that improves the energy conservation in the low Mach number limit, as well as the treatment of gravity waves (we explore this for a variety of problems in A. S. Almgren et al. 2013, in preparation). We note, however, that this additional term has little effect in a convective layer, but we include it for completeness.

Table 1
ReacLib Reaction Rates Used in Approximate Network

| Reaction | ReacLib Reference Label |
|----------|------------------------|
| $^{14}$O($p, \gamma$)$^{15}$N | $^{15}$N$_0$9 |
| $^{14}$N($p, \gamma$)$^{15}$O | $^{15}$O$_{im05}$ |
| $^{15}$O($e^+, \gamma$)$^{16}$N | $^{16}$N$_{wc07}$ |
| $^{15}$O($\alpha, p$)$^{16}$F | $^{16}$F$_{He06}$ |
| $^{15}$O($e^+, \gamma$)$^{15}$N | $^{15}$N$_{wc07}$ |
| $^{15}$O($\alpha, \gamma$)$^{18}$Ne | $^{18}$Ne$_{dc11}$ |
| $^{16}$O($\alpha, \gamma$)$^{20}$Ne | $^{20}$Ne$_{co10}$ |
| $^{16}$O($p, \gamma$)$^{15}$F | $^{15}$F$_{ia08}$ |
| $^{17}$F($e^+, \gamma$)$^{18}$O | $^{18}$O$_{wc07}$ |
| $^{17}$F($\gamma, p$)$^{18}$O | $^{18}$O$_{ia08}$ |
| $^{17}$F($p, \gamma$)$^{18}$Ne | $^{18}$Ne$_{cb09}$ |
| $^{18}$Ne($e^+, \gamma$)$^{19}$F | $^{19}$F$_{wc07}$ |
| $^{18}$Ne($\alpha, p$)$^{21}$Na | $^{21}$Na$_{mv09}$ |
| $^{19}$Ne($e^+, \gamma$)$^{20}$F | $^{20}$F$_{wc07}$ |
| $^{20}$Ne($p, \gamma$)$^{21}$Na | $^{21}$Na$_{il10}$ |
| $^{20}$Ne($\alpha, p$)$^{23}$P | $^{23}$P$_{th38}$ |
| $^{21}$Ti($\alpha, p$)$^{23}$V | $^{23}$V$_{rh10}$ |
involve competition between a $\beta^+$ decay of an isotope of Ne and an $(\alpha, p)$ or $(p, \gamma)$ reaction with branching ratios given by $\lambda_1$ or $\lambda_2$, respectively. For example, the chain of reactions $^{15}\text{O}(\alpha, \gamma)^{19}\text{Ne}(p, \gamma)^{20}\text{Na}(p, \gamma)^{21}\text{Mg}(\beta^+)^{21}\text{Na}(p, \gamma)^{22}\text{Mg}$ is approximated as turning $^{15}\text{O}$ (plus an $\alpha$ and three protons) directly into $^{22}\text{Mg}$ at a rate governed by the $\alpha$ capture on $^{15}\text{O}$ multiplied by the fraction $(1 - \lambda_2)$ of $^{19}\text{Ne}$ isotopes that proton capture before they $\beta^+$ decay. At the high temperatures and densities experienced during an XRB, many of the $\beta^+$-decay waiting points of the traditional rp process are bypassed via $(p, \gamma)$ and/or $(\alpha, p)$ reactions. For the flow in the rp process up through $^{56}\text{Ni}$, the approximate network accounts for these bypassing reactions by assuming all reactions pass through the fastest path. For example, converting $^{22}\text{Mg}$ to $^{30}\text{S}$ can proceed through two main channels: (1) a series of eight $p$-captures and several $\beta^+$ decays, or (2) two $(\alpha, p)$ and two $(p, \gamma)$ reactions. The faster of the two paths will be used by the network. However, each individual path is limited by its slowest rate. For the first path—the $\beta^+$-decay path—the limiting factor is the mean lifetime of the $\beta^+$ decays; the second path is limited by the slower of the two $\alpha$-capture rates, namely $^{28}\text{Si}(\alpha, p)^{30}\text{P}$. Likewise, burning $^{30}\text{S}$ to $^{56}\text{Ni}$ in the approximate network is restricted by a typical $\beta^+$-decay timescale or $\alpha$ capture on $^{44}\text{Ti}$. Finally, $^4\text{He}$ burning via the triple-$\alpha$ reaction enters the diagram from the bottom left corner. A general stellar equation of state with ideal ions, arbitrarily degenerate/relativistic electrons, and radiation is used (Timmes & Swesty 2000). Paper I showed that including thermal diffusion did not significantly alter the average properties of the convection or the maximum temperature reached during the simulation. Consequently, we neglect thermal diffusion in the calculations of this paper. Malone et al. (2011) also discussed a volume discrepancy factor that is designed to drive the flow back onto the constraint dictated by the equation of state. For the present simulations we run with this off (equivalent to $f = 0$ in Equation (13) of Malone et al. 2011).

To assess the validity of the approximate network we perform a one-zone, constant pressure, self-heating burn using the conditions similar to those at the base of the accreted layer in an XRB: $T = 9.5 \times 10^8 \text{ K}$, $\rho = 5.93 \times 10^6 \text{ g cm}^{-3}$, $X(^1\text{H}) = 0.72$, $X(^4\text{He}) = 0.24$, and the remaining abundance split between $^{14}\text{O}$ and $^{15}\text{O}$ in a ratio comparable to their respective $\beta^+$-decay times. The solid lines in Figure 2 show the early evolution of the hydrogen/helium abundance (top), specific energy generation rate (middle), and temperature (bottom) for our approximate network. The dotted lines show a comparison of a simple calculation with the same initial conditions but using an adaptive reaction network from the Kepler code-base, which included many nuclei up to Ge. The two networks agree quite well under these conditions, but the approximate network initially tends to be $\lesssim 10\%$ hotter than the larger Kepler network.
3. INITIAL MODEL AND SIMULATION PARAMETERS

We generate parameterized models of the accreted layer using simulations run by the Kepler stellar evolution code as a guide. Creating our own models alleviates the difficulty of reproducing the proper convectively unstable regions in the atmosphere of the one-dimensional model. In particular, mapping from a Lagrangian grid to an Eulerian grid, interpolating data to a constant mesh spacing, and slight differences in the thermodynamics between codes can all lead to differences in thermal/adiabatic gradients, and hence which region is convectively unstable. Additionally, spurious features in the one-dimensional model can cause difficulties while mapping onto an Eulerian grid and maintaining HSE, especially in regions of sharp discontinuities in the Lagrangian code.

Our simplified models and their generation are described in detail in the Appendix. Briefly, our models consist of a 1.4 $M_\odot$, 10 km, isothermal ($T = T_{\text{ns}}$) “neutron star” substrate composed of heavy elements ($X = X_{\text{ns}} \equiv$ pure $^{56}$Ni) with a warm accreted layer of mixed fuel composition ($X = X_{\text{fuel}}$), part of which is convectively unstable with an isentropic gradient. The transition between the neutron star and the accreted layer is governed by the density ($\rho_{\text{base}}$) and temperature ($T_{\text{base}}$) at the base of the accreted layer. The composition of the accreted layer was approximated from an initial Kepler XRB model, but is essentially a slightly metal-rich gas compared to solar metallicity—to reflect prior burning—with the $^{15}$O/$^{14}$O ratio set approximately by their respective lifetime against $\beta^-$ decay. Table 2 gives the set of parameters that describe the models—refer to the Appendix for the definitions.

Our first attempt at model creation used values of $\rho_{\text{base}}$ ($\sim 7 \times 10^8$ g cm$^{-3}$) and $T_{\text{base}}$ ($\sim 7.5 \times 10^8$ K) determined from the original Kepler models. When mapped into two dimensions, these models exhibited weaker burning than their one-dimensional counterparts. This leads to a slowly increasing base temperature that eventually peaked around $\lesssim 10^9$ K, and then remained roughly constant. As we found in Paper I with semi-analytic models, the multidimensional convection generated in these models was much more efficient at carrying heat than the mixing length theory prescription used in the one-dimensional Kepler models.

To create more prolific burning, we therefore modified our initial conditions to those given in Table 2. Namely, we artificially increased the density to $\rho_{\text{base}} = 2 \times 10^9$ g cm$^{-3}$ and the temperature to $T_{\text{base}} = 9.5 \times 10^8$ K while keeping the composition fixed. Increasing the temperature and density has two main consequences for the burning in the layer: (1) boosting the triple-$\alpha$ reaction ($\propto \rho^3$), which is temperature sensitive, relative to the $\beta$-limited HCNO cycle, and (2) decreasing the branching ratios $\lambda_1$ and $\lambda_2$ (see Figure 1), which allows for an increase in breakout from the HCNO cycle. Ultimately, this quicker consumption of $^4$He nuclei early on will slow the late-time evolution of the burning as ($\alpha, \beta^-$) reactions might not be frequent enough to bridge $\beta^+$-decay waiting points. However, our burning does not reach that far into heavy elements so we are not concerned with this aspect here. Figure 3 shows the initial density, temperature and bulk composition profiles for the model used in our calculations.

| Parameter | Value |
|-----------|-------|
| $\rho_{\text{base}}$ | $2 \times 10^9$ g cm$^{-3}$ |
| $T_{\text{ns}}$ | $3 \times 10^8$ K |
| $T_{\text{base}}$ | $9.5 \times 10^8$ K |
| $T_{\text{cutoff}}$ | $5 \times 10^7$ K |
| $H$ | 1450 cm |
| $\delta$ | 12.0 cm |
| $g$ | $-2.45 \times 10^{14}$ cm s$^{-2}$ |

Table 2

Initial Model Parameters

| Fuel composition, $X_{\text{fuel}}$ | Value |
|----------------------------------|-------|
| $^1$H | 0.72 |
| $^4$He | 0.24 |
| $^{14}$O | $4 \times 10^{-4}$ |
| $^{15}$O | $3 \times 10^{-3}$ |
| $^{22}$Mg | $10^{-3}$ |
| $^{38}$S | $10^{-3}$ |
| $^{56}$Ni | 0.0346 |

| Neutron star composition, $X_{\text{ns}}$ | Value |
|-----------------------------------------|-------|
| $^{56}$Ni | 1.0 |

Figure 3. Initial one-dimensional model for the simulations of this paper. The vertical gray lines indicate the radial position of the start of the sponge ($r = r_{\text{sponge}}$); leftmost line) and the cutoff density/anelastic cutoff ($r = r_{\text{min}}$); rightmost line).

(A color version of this figure is available in the online journal.)
As with our simulations of convection in/on white dwarfs (Zingale et al. 2013; Nonaka et al. 2012), and also in Paper I, we use a low density cutoff and a sponging technique to control the behavior of the flow at the top of the atmosphere. These are designed to suppress unwanted velocities in the region above our accreted layer. The low density cutoff acts to change the behavior of the low Mach number algorithm when the density drops below a certain value. In particular, when the density drops below \( \rho_{\text{anel}} \), the divergence constraint on the velocity field is altered to resemble that of the anelastic approximation, \( \nabla \cdot (\rho_0 U) = 0 \). There is another low density cutoff, \( \rho_{\text{cutoff}} \), that is the density at which we fix the ambient medium. Both \( \rho_{\text{anel}} \) and \( \rho_{\text{cutoff}} \) are runtime parameters, which we set to \( \rho_{\text{cutoff}} = \rho_{\text{anel}} = 10^3 \text{ g cm}^{-3} \) in the present simulations. The location where the density first drops below the cutoffs is shown as the rightmost thin vertical gray line in Figure 3.

For the sponge, we pick a multiple, \( f_{\text{sp}} \), of the anelastic cutoff to define the density at which the sponge turns on, \( \rho_{\text{sp}} = f_{\text{sp}} \rho_{\text{anel}} \). The sponge is designed to be in full force when the density drops below \( \rho_{\text{anel}} \), the divergence constraint on the velocity field. For the sponge, we pick a multiple, \( f_{\text{sp}} \), of the anelastic cutoff to define the density at which we fix the ambient medium.

\[
\rho_{\text{anel}} = \begin{cases} 
1, & \text{if } r < \rho_{\text{sp}} \\
\frac{1}{2} (1 - s_{\text{min}}) \cos \left( \frac{\pi (r - \rho_{\text{anel}})}{\rho_{\text{anel}} - \rho_{\text{sp}}} \right) + \frac{1}{2} (1 + s_{\text{min}}), & \text{if } \rho_{\text{sp}} \leq r < \rho_{\text{anel}} \\
s_{\text{min}}, & \text{otherwise.}
\end{cases}
\]

(1)

and after the velocity is advanced, the sponge is applied as

\[
U^{n+1} \rightarrow sU^{n+1}.
\]

(2)

For all the simulations presented here, we choose \( f_{\text{sp}} = 25 \) and \( s_{\text{min}} = 0.01 \). The leftmost vertical gray line in Figure 3 marks the location of the sponge start, \( \rho_{\text{sp}} \) (i.e., where \( \rho = f_{\text{sp}} \rho_{\text{anel}} \)).

To seed the convection, we add a number, \( n_{\text{vort}} \), of small vortices to the initial conditions at a fixed height, \( r_{\text{vort}} \), near the base of the convective region. The vortices are spaced equally across the domain, and the orientation—clockwise versus counterclockwise—is altered every other vortex. Each vortex is Gaussian in form with the velocity perturbations.

\[
\delta u_i(x, r) = - (-1)^i A_{\text{vort}} (r - r_{\text{vort}}) \exp \left( -\frac{d_i^2}{\sigma^2} \right),
\]

\[
\delta v_i(x, r) = (-1)^i A_{\text{vort}} (x - x_{\text{vort},i}) \exp \left( -\frac{d_i^2}{\sigma^2} \right),
\]

where \( u \) and \( v \) are the horizontal and vertical components of the velocity, respectively, \( A_{\text{vort}} \) is the amplitude of the perturbation, \( (x_{\text{vort},i}, r_{\text{vort}}) \) is the center of the \( i \)th vortex, \( d_i = [(x - x_{\text{vort},i})^2 + (r - r_{\text{vort}})^2]^{1/2} \) is the distance from the center of \( i \)th vortex, and \( \sigma \) is the size of the vortex. The superposition of all vortices is used to determine the initial velocity field, that is,

\[
(u, v) = \left( \sum_{i=1}^{n_{\text{vort}}} \delta u_i, \sum_{i=1}^{n_{\text{vort}}} \delta v_i \right).
\]

(3)

For the simulations presented here, we choose \( r_{\text{vort}} = 1475 \text{ cm}, A_{\text{vort}} = 1 \text{ km s}^{-1}, \sigma^2 = 200 \text{ cm}^2 \), and \( n_{\text{vort}} = 16 \) (each \( x_{\text{vort},i} \) is determined from the domain width and \( n_{\text{vort}} \)). We note that the initial convective region for this model roughly spans the region between \( 1470 \text{ cm} \lesssim r \lesssim 3350 \text{ cm} \).

4. RESULTS

We perform simulations at three resolutions: 12, 6, and 3 cm zone\(^{-1} \). The 12 and 6 cm runs are done with a uniform grid. For the 3 cm run, we added a single level of refinement to the 6 cm model in a region encompassing the convective zone. We do not dynamically change the grid with time; this allows us to optimize the load balancing of the simulation. Each of these simulations used a two-dimensional grid of size 1536 cm \( \times \) 4608 cm. A double-wide model at 6 cm zone\(^{-1} \) resolution was also created and mapped onto a grid of 3072 cm \( \times \) 4608 cm. This fourth model comprises the bulk of the study in this paper, as it was evolved the furthest in time.

All simulations here assumed plane-parallel geometry with a constant gravitational acceleration of \( g = -2.45 \times 10^{14} \text{ cm s}^{-2} \). Periodic boundary conditions were used in the lateral, or \( x \) direction. The vertical, or \( r \)-direction, upper boundary was an outflow boundary while the lower boundary used slip-wall conditions.

4.1. General Trends and Resolution Dependence

As in our simulations of Paper I, a transient event occurs at the onset of convective overturn. This transient causes relatively large velocity spikes until the system adjusts to a more steady-state convective flow field. Based on our experience in previous studies of convection with Maestro (Nonaka et al. 2012; Zingale et al. 2013), including an initial velocity perturbation, such as that in Equation (3), helps to minimize the transient by giving the system a small “kick,” allowing the energy to be more quickly dispersed via advection. This is different from the approach of Paper I where we let solver noise seed convection. After a few turnover times (\( \lesssim 10^{-3} \) s), however, the convective pattern does not remember how it was initiated; therefore, the results presented here are not sensitive to the choice of initial perturbations.

Figure 4 shows the peak Mach number, \( M \), in the domain as a function of time for all four of our models. At very early time, the Mach number peaks to about 0.18 for all simulations because of the transient discussed above. By about \( t = 0.01 \) s, the system has relaxed to a steady-state convective flow. While the 12 cm zone\(^{-1} \) run differs markedly from the others, the 3 and 6 cm zone\(^{-1} \) runs appear to be converged. Also, note that the Mach number is generally smaller for the higher-resolution runs. We suspect that the primary source of the differences with resolution is in the reaction source term. The energy generation is strongly peaked near the base of the burning layer, and, as a result, a coarse simulation will underestimate the total energy generation (since the coarse-zone cell center is at a lower temperature than the fine-zone cell center at the base of the layer). This was also discussed in Paper I in the context of pure triple-\( \alpha \) burning, which required a very fine spatial resolution due to its high temperature sensitivity. Also similar to the results of Paper I, the time-averaged peak velocity remains less than 10% of the sound speed, validating the use of a low Mach number approximation method for XRBs.

Similarly, Figure 5 shows the peak temperature in the domain as a function of time for all four runs. Again, we see—excluding the 12 cm zone\(^{-1} \) run—the temperature evolution of the models is quite similar, agreeing to within \( \lesssim 5\% \).
Figure 4. Resolution study showing the maximum Mach number on the grid. There is good agreement between the 3 and 6 cm zone$^{-1}$ models, suggesting that we are nearly converged. We also see that peak Mach number systematically decreases with increasing resolution, likely due to better capturing of the peak of burning at the base of the accreted layer. (A color version of this figure is available in the online journal.)

In addition to underestimating the energy generation, the coarse model with 12 cm zone$^{-1}$ resolution also tends to overestimate the amount of convective overshoot. This can also be inferred from Figure 4; the overall larger velocities allow for parcels of fluid on ballistic trajectories to more readily penetrate the convective boundary, thereby increasing the heat flux away from the base of the accreted layer and increasing the rate at which it can cool.

Of the three different resolutions we tested, the 6 cm zone$^{-1}$ simulations offer the best tradeoff between accuracy and computational cost. The narrow-domain 6 cm zone$^{-1}$ model, however, has a domain width comparable to the initial vertical extent of the convective region. This forces the convective rolls to assume an aspect ratio $\lesssim 1$, which alters the dynamics and allows for the $\lesssim 30\%$ difference in the time-averaged $M$ between the normal 6 cm zone$^{-1}$ model and the wide model. The double-wide domain alleviates the aspect ratio forcing for the duration of the simulations presented here. Therefore, we focus on the 6 cm zone$^{-1}$ wide-domain simulation for the remainder of this paper.

4.2. Convection in the Wide Domain

4.2.1. Early Adjustment

Figure 6 shows the transient adjustment phase discussed in Section 4.1, as seen in three different variables: magnitude of vorticity (left column), Mach number (middle column), and specific energy generation rate (right column). The initial conditions are in the top row; note that the vortices of Equation (3) are just barely discernible on the vorticity color scale. After $3 \times 10^{-3}$ s (middle row), the nonlinear interactions of the perturbations give rise to a handful of dominant plumes that provide the large Mach number of the transient startup. Another $3 \times 10^{-4}$ s later ($t = 6 \times 10^{-4}$ s; bottom row) and the convective pattern has fully filled the region that was originally Schwarzschild-unstable in the initial model. We see localized vortices, and where the flow converges near the bottom of the convective layer, we also have a localized increased burning rate.

4.2.2. Well-defined Convection Region

Figure 7 shows the same evolution as Figure 6, except at later times ($5 \times 10^{-3}$, $5 \times 10^{-2}$, $10^{-1}$, and $2 \times 10^{-1}$ s, from top to bottom). As is well known in two-dimensional simulations, smaller vortices tend to merge into larger vortices. Some of the smaller-scale features are smoothed out and the burning becomes (laterally) very uniform within the burning region. It is also clear from Figure 7 that the convective region expands both radially inward and outward, with the extent of the former being much less than that of the latter.

The expansion of the convectively unstable region can also be seen by looking at the Brunt–Väisälä or buoyancy frequency, $N$, for a stratified atmosphere (see, for example, Chapter 6 in Kippenhahn & Weigert (1992)):

$$N^2 = -g \left( \frac{d \ln \rho}{dr} - \frac{d \ln \rho}{dr}_{\text{ad}} \right),$$

where the subscript “ad” means along an adiabat, and we are assuming instability to Schwarzschild convection. Equation (4) gives the square of the frequency at which a fluid element will oscillate if displaced from its equilibrium position ($\propto e^{iNt}$). When $N^2 < 0$, then the buoyancy frequency is purely imaginary, giving rise to an instability. Figure 8 shows profiles of the square of the Brunt–Väisälä frequency as calculated from the laterally averaged quantities—i.e., with the gradients in Equation (4)
Figure 6. Early adjustment of the system shown in magnitude of vorticity (left), Mach number (middle), and logarithm of the specific energy generation rate (right) at $t = 0$ s, $3 \times 10^{-3}$ s, and $6 \times 10^{-4}$ s from top to bottom. By $t \sim 5 \times 10^{-4}$ s, the flow pattern has filled the entire convective region. Note the presence of a secondary local maximum in energy generation rate in the initial conditions around $r \sim 2400$ cm.

(A color version of this figure is available in the online journal.)

being calculated as

$$\frac{d \ln \rho}{dr} \rightarrow \frac{d \ln \langle \rho \rangle}{dr}$$

and

$$\left| \frac{d \ln \rho}{dr} \right|_\text{ad} \rightarrow \frac{d \ln \rho \langle \langle p \rangle, \langle T \rangle, \langle X \rangle \rangle}{dr} \bigg|_\text{ad},$$

where angle brackets denote laterally averaged quantities. The different curves are, from top to bottom, profiles at $t = 5 \times 10^{-3}$, $5 \times 10^{-2}$, $10^{-1}$, and $2 \times 10^{-1}$ s, each being offset for clarity. The regions of instability ($N^2 < 0$) for each curve have been highlighted red.

In an average sense, the upper boundary of the convective region pushes radially outward, consistent with the color map plots of Figure 7. However, at any given instance, the tenuous material just outside the upper convective boundary gives rise to fluctuations in entropy (or $N^2$) that make a sharp distinction of the boundary difficult. Indeed, the plots of $N^2$ at the upper boundary have much more noise than at the lower boundary, where there exists a sharp transition between neutron star and atmosphere. The lower boundary is always marked by a large (positive) $N^2$. This results in stable displacements of fluid elements that give rise to internal gravity waves, such as the wave-like features at the base of the convective region in the plots of energy generation in Figure 7.

A peculiar feature evident in Figure 8 at late time (bottom curve) is a small region of convective stability around $r = 2850$ cm that splits the single convective zone into two layers of convection. This can be seen in either the vorticity or Mach.
Figure 7. Convective evolution of magnitude of vorticity (left), Mach number (middle), and logarithm of the specific energy generation rate (right) at $t = 5 \times 10^{-3}$ s, 5 $\times$ $10^{-2}$ s, 10$^{-1}$ s, and $2 \times 10^{-1}$ s from top to bottom. The secondary peak in energy generation rate tends to dominate the burning after $\sim 10^{-1}$ s of evolution, and the convective region splits into layers shortly thereafter.

(A color version of this figure is available in the online journal.)
The lateral average. Note that as time progresses, the second peak in shows the lateral average at a given radius plus or minus the rms deviation from relatively more prominent and moves further out in the atmosphere.

Looking back at the initial conditions for the energy generation rate in the top row of Figure 6, we see that indeed there is a secondary, weaker peak above the base of the atmosphere. This peak tends to strengthen with time, while the peak of burning at the base of the accreted layer weakens (as seen in Figures 6 and 7). Figure 9 shows the lateral average (±1σ) of the energy generation rate at the same time as the snapshots in Figure 7. By t = 10^{-1} s, the two peaks have comparable energy output, while at later times what was initially the secondary peak slightly dominates the burning at the base of the accreted layer. The secondary peak also appears to move radially outward in the atmosphere at about the same rate as the expansion of the convective zone ~60 m s^{-1}.

The presence of the secondary peak is a feature strengthened by the approximations in the network used here. In general, in the accreted layer, the density and temperature are decreasing functions of radius. How, then, can a constant composition profile produce a non-monotonic energy generation rate profile? The answer lies in the branching ratio between the rp-process breakout and returning to the HCNO cycle in the approximate network. In particular, for the initial conditions, Figure 10 shows in blue the branching ratio, λ_1, which was defined in Figure 1 as the fraction of ^{18}Ne that β^+ decays to ^{18}F faster than it can α capture. The β^+ -decay rate is—for lack of better physics of T-dependent weak decays—a constant, whereas the α capture has to overcome a Coulomb barrier. This causes λ_1 to increase with decreasing temperature, and we see a sharp transition in the branching ratio around r ≈ 2200 cm. Note that the branching ratio is unity in the neutron star substrate as there is no ^{4}He available for capture on ^{18}Ne. Also shown in Figure 10 in red is the normalized rate at which ^{17}F (plus a proton) is converted directly to ^{15}O (plus an α; red) in the approximate network. This approximate reaction chain is responsible for the secondary peak in energy generation rate seen in Figures 6, 7, and 9, and the split of the convective region into two layers.

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The branching ratio

Figure 11. Density, temperature, and various species profiles both at the start (dashed lines) and end (solid lines) of the simulation for the wide 6 cm$^{-1}$ model. The density and temperature profiles show just how much the atmosphere has expanded during the burn. The composition profiles show both regions of convective overshoot (relatively large abundances below $r \sim 1500$ cm), as well as the split in convective layers around $r \sim 2800$ cm.

Figure 12. Evolution of the total mass for each species normalized to its starting value. The inset plot shows a zoom in on the last 10 ms of evolution and uses a linear scale. $^{16}$O and $^{17}$F were out of equilibrium due to approximations made in constructing the initial model. The total production of $^{56}$Ni from $^{30}$S is negligible. The total amount of $^4$He and $^1$H burned by mass was $\lesssim 27\%$ and $\lesssim 1.5\%$, respectively.

(A color version of this figure is available in the online journal.)
5. DISCUSSION AND CONCLUSIONS

We presented the first multidimensional calculations of convective flow in the context of mixed H/He XRBs using realistic hydrodynamics and an approximate reaction network for H/He burning. We demonstrated convergence of our results and explored the behavior of the nucleosynthesis and convection. The approximate network we utilized assumed that some reaction chains occurred faster than what would happen in a larger network.

In addition, the approximate network utilized here resulted in the development of two layers of convection as a result of the existence of a secondary peak in energy generation rate, which eventually dominated the total energy output. We traced the cause of this secondary peak in energy generation rate to the critical rp-process breakout branching ratio, \( \lambda_1 \), which measures the ratio of the \( \beta^+ \) -decay rate versus \( \alpha \)-capture rate of \(^{18}\)Ne. With our particular initial conditions, this branching ratio sharply transitions between zero and one midway through our atmosphere.

The secondary peak in energy generation rate becomes comparable to the primary peak around \( t \sim 0.1 \) s (see Figure 9). The split of the convective region lags behind the growth of the energy generation rate peak. Indeed, the two-layered structure is not well defined until about \( t \sim 0.14 \) s. A small entropy jump between the two layers prevents material from crossing between each layer. This causes a quenching of the mixing of isotopes and alters the burning. Coincidentally, Figure 5 shows that the rate of increase of the peak temperature changes around the time of layer formation.

We note that we artificially boosted the temperature and density at the base of our accreted layer to give prodigious burning (see the discussion in 3). Simple Kepler calculations show that in order to reproduce a model with characteristics similar to our base density, the initial metallicity of the accreted material has to be turned down significantly, \( Z \sim 10^{-4} \), making such a system perhaps rare in nature. Continuing these calculations in one dimension, the full network in Kepler showed a very slight non-monotonicity of the energy generation rate in a region containing composition profiles qualitatively similar to what we see near the development of our secondary peak in the energy generation rate. However, this minor bump in Kepler's energy generation rate was transient and certainly never dominated the burning as we see in our calculations with the approximate network. The development of layered convective regions in our simulations is likely artificial and due to the approximations used in the reaction network.

These calculations are a starting point for more realistic calculations of H/He XRBs. Future work will focus on improving the nuclear physics, moving to three dimensions, and considering larger domains. We note that very little hydrogen and helium were processed during the short duration of our simulations—and similar Kepler calculations show very little change in energy generation rate profiles on this timescale. This suggests that even further (and possibly more accurate) simplifications can be made to the network for use on the short timescales amenable to multidimensional simulations. Indeed, the original approximate network of Wallace & Woosley (1981) was designed (in part) to model the full burst cycle where copious amounts of heavy elements were produced. Improvements to the nuclear physics and approximations therein are work for a future paper.

In addition, one path that will enable larger simulations is to develop a subgrid model for the burning, and using more realistic initial models (perhaps following the methodology from Cumming & Bildsten 2000, or better mapping techniques between Kepler and Maestro models). It seems that we can capture the convective behavior on a medium-resolution grid, but the steep temperature dependence in the reactions requires finer resolution for the energy generation peaks. This was much more extreme in the case of pure He bursts (Paper I) than in the calculations here; however, a potential path forward is to use subgrid resolution for the burning and average the resulting energetics and compositions back to the hydrodynamic grid. Ultimately, we would like to model a laterally propagating burning front with realistic nuclear physics. In the context of Maestro, this will require support for lateral gradients instead of a single base state. This development will be explored in tandem with the follow-up simulations described above.

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APPENDIX

INITIAL MODELS

We define our parameterized models to consist of three regions: an isothermal lower region, representing the underlying neutron star; a ramp-up region to bring us up to the temperature at the base of the accreted layer; and an isentropic region at the surface, which is where the convection will take place.

We specify the temperature in the lower isothermal region, \( T_{\text{ns}} \); the temperature at the base of the accreted layer, \( T_{\text{base}} \); the density at the base of the accreted layer, \( \rho_{\text{base}} \); the width of the transition region, \( \delta \); and the lowest temperature in the convection region, \( T_{\text{cutoff}} \). Additionally, we specify the composition in the accreted layer, \( X_{\text{fuel}} \), and the composition in the underlying neutron star, \( X_{\text{ns}} \). For all these calculations, we hold the gravitational acceleration, \( g \), constant. The basic procedure follows the methodology outlined in Zingale et al. (2002).

We set the start of the base of the accreted layer a distance \( H \) from the bottom of the domain. The temperature and composition are set to

\[
X_t = X_{\text{fuel}} + \frac{1}{2}(X_{\text{fuel}} - X_{\text{ns}}) \left[ 1 + \tanh \left( \frac{T_t - T_{\text{cutoff}}}{\delta} \right) \right]
\]
\[ T_i = T_{\text{base}} + \frac{1}{2}(T_{\text{base}} - T_{\text{ns}}) \left[ 1 + \tanh \left( \frac{r_i - H}{\delta} \right) \right]. \] (A2)

This temperature serves as an initial guess in the isentropic region and will be reset there.

We choose the base of the accreted layer as the starting point of integration. We determine the base pressure and entropy to find the needed pressure, the Maestro source release in MAESTRO

\[ p_{\text{base}} = p(\rho_{\text{base}}, T_{\text{base}}, X_{\text{fuel}}); \quad s_{\text{base}} = s(\rho_{\text{base}}, T_{\text{base}}, X_{\text{fuel}}). \] (A3)

We integrate radially outward from the base, using the condition of hydrostatic equilibrium to find the needed pressure. We then use the Newton–Raphson method to correct the pressure to that demanded by HSE.

1. Pick an initial guess for \( \rho_i \) and \( T_i \).
2. Compute the hydrostatic pressure

\[ p_i^{\text{HSE}} = p_{i-1} + \frac{1}{2} \Delta r (\rho_i + \rho_{i-1}) g. \] (A4)

3. Define

\[ F = p_i^{\text{HSE}} - p_i^{\text{EOS}}, \quad G = s_i^{\text{HSE}} - s_i^{\text{EOS}}, \] (A5)

where \( p_i^{\text{EOS}} = p(\rho_i, T_i, X_{\text{fuel}}) \) and \( s_i^{\text{EOS}} = s(\rho_i, T_i, X_{\text{fuel}}) \) from the equation of state. We then use the Newton–Raphson method to correct \( \rho_i \) and \( T_i \) subject to \( F = G = 0 \).

4. We continue to iterate on this zone until we converge.

If the temperature falls below \( T_{\text{cutoff}} \), we switch to constraining only the hydrostatic pressure, keeping the temperature constant.

This defines the isentropic region above the base of the accreted layer. Beneath the base (including the transition region characterized by width \( \delta \)), we integrate radially inward, constraining the pressure to that demanded by HSE,

\[ p_i^{\text{HSE}} = p_{i+1} - \frac{1}{2} \Delta r (\rho_i + \rho_{i+1}) g. \] (A7)

Since we are using the prescribed temperature, we only need to zero \( F \equiv p_i^{\text{HSE}} - p_i^{\text{EOS}} \) using the Newton–Raphson technique.

The code to generate these initial models is provided in the Maestro source release in MAESTRO/Util/initial_models/toy_atm.