THE INITIATION AND PROPAGATION OF HELIUM DETONATIONS IN WHITE DWARF ENVELOPES

KEN J. SHEN1,3 AND KEVIN MOORE2

1 Department of Astronomy and Theoretical Astrophysics Center, University of California, Berkeley, CA 94720, USA; kenshen@astro.berkeley.edu
2 Department of Applied Mathematics and Statistics, University of California, Santa Cruz, CA 95064, USA

Received 2014 September 11; accepted 2014 October 14; published 2014 November 24

ABSTRACT

Detonations in helium-rich envelopes surrounding white dwarfs have garnered attention as triggers of faint thermonuclear “Ia” supernovae and double detonation Type Ia supernovae. However, recent studies have found that the minimum size of a hotspot that can lead to a helium detonation is comparable to, or even larger than, the white dwarf’s pressure scale height, casting doubt on the successful ignition of helium detonations in these systems. In this paper, we examine the previously neglected effects of C/O pollution and a full nuclear reaction network, and we consider hotspots with spatially constant pressure in addition to constant density hotspots. We find that the inclusion of these effects significantly decreases the minimum hotspot size for helium-rich detonation ignition, making detonations far more plausible during turbulent shell convection or during double white dwarf mergers. The increase in burning rate also decreases the minimum shell mass in which a helium detonation can successfully propagate and alters the composition of the shell’s burning products. The ashes of these low-mass shells consist primarily of silicon, calcium, and unburned helium and metals and may explain the high-velocity spectral features observed in most Type Ia supernovae.

Key words: binaries: close – nuclear reactions, nucleosynthesis, abundances – supernovae: general – white dwarfs

1. INTRODUCTION

He-rich accretion onto a white dwarf (WD) can, for the right range of parameters, lead to the formation of a supersonic He-burning detonation in the accreted shell. While it was first suggested over 30 yr ago that the He detonation can trigger a core detonation and subsequent Type Ia supernova (SN Ia; e.g., Woosley et al. 1980; Nomoto 1982), this “double detonation” scenario fell mostly out of favor for years. However, interest in the scenario has been rekindled in the past decade (Fink et al. 2007, 2010; Sim et al. 2010, 2012; Kromer et al. 2010; Ruiter et al. 2011, 2014; Moll & Woosley 2013; Dan et al. 2014), in part due to the possibility that the progenitor system is a double WD binary in which the He detonation occurs during a convective shell-burning phase (Bildsten et al. 2007; Shen & Bildsten 2009) or during the initial stages of a merger (Guillochon et al. 2010; Raskin et al. 2012; Pakmor et al. 2013). The double detonation scenario is able to match observed SN Ia rates (Maoz et al. 2011; Ruiter et al. 2011, 2014) and avoid unobserved effects that a large non-degenerate binary companion would impart on the SN Ia’s light curve and spectra (Kasen 2010; Bloom et al. 2012; Schaefer & Pagnotta 2012). While recent observations of circumstellar material in ~20% of SNe Ia (Patat et al. 2007; Sternberg et al. 2011, 2014; Maguire et al. 2013) have been used as evidence for a single degenerate scenario (Patat et al. 2011; Moore & Bildsten 2012), these signatures can also be produced during double WD binary evolution (Raskin & Kasen 2013; Shen et al. 2013).

In recent years, it has been suggested that He shell detonations are possible in small shells that might not trigger core detonations and SNe Ia, especially if the donor is a low-mass He WD for which the accretor’s convective He-burning shell is \( \lesssim 0.1 M_\odot \). While subsequent work finds that even detonations in these small He shells will trigger detonations in C/O cores \( \gtrsim 0.8 M_\odot \), O/Ne and lower-mass C/O cores may remain intact (Shen & Bildsten 2014). The resulting explosion of only the He shell would be a faint and rapidly evolving “Ia” SN (Bildsten et al. 2007; Shen & Bildsten 2009; Shen et al. 2010; Waldman et al. 2011). These “Ia” SNe have been suggested as possible explanations for the newly discovered classes of SNe Iax (see Foley et al. 2013 for an overview), Ca-rich/O-poor transients (Perets et al. 2010; Kasliwal et al. 2012), and rapidly fading SNe Ia (e.g., Perets et al. 2011; Drout et al. 2014).

The possibility of double detonations and “Ia” SNe is predicated on the successful ignition and propagation of the He detonation. Initial estimates assumed ignition occurs when the local He-burning timescale becomes shorter than the local dynamical timescale, \( t_{\text{dynamical}} = H/c_s \), where \( H \) is the pressure scale height and \( c_s \) is the sound speed (Bildsten et al. 2007; Shen & Bildsten 2009; Guillochon et al. 2010; Dan et al. 2014). However, this is equivalent to assuming that material encompassing the entire scale height is involved in the initiation of the He detonation, so that the timescale for the growing overpressure to expand is the time for sound waves to traverse the scale height. In actuality, the He detonation is triggered in a very small region within the WD’s envelope, so that the actual dynamical timescale of interest is the much shorter sound crossing time of this subregion.

As a result, more recent studies such as Holcomb et al. (2013) quantifying the necessary conditions for He ignition have found that triggering a He detonation is instead prohibitively difficult. They found that detonations arising from perturbed hotspots require hotspots comparable in size to the WD’s scale height. Given the improbability of generating a stochastic fluctuation as large as this, these studies implied that He detonations do not occur on WDs.

However, because their work was an initial exploration, Holcomb et al. (2013) assumed a pure He composition for their calculations. In reality, the He layer will be polluted with a non-negligible fraction of C/O. In the case of He detonations...
triggered during a double WD merger, such pollution occurs due
to dynamical mixing between the direct impact accretion stream
and the accretor’s core. For convectively ignited He detonations,
the convective fluid motions prior to the detonation may shear
cross the composition discontinuity between the He shell and
C/O core and dredge up core material, in close analogy to metal-enriched
classical nova ejecta (Gehrz et al. 1998). Furthermore, a
C/O mass fraction of 5%–10% is generated by the previous He-
burning phase prior to the onset of dynamical burning (Shen &
Bildsten 2009). In addition to 12C and 16O, the accreted material
will also contain a significant amount of 14N, since this isotope
is the slowest point of the CNO cycle and will be present in the
He-rich material that has undergone prior CNO H-burning.

As we demonstrate in Section 2, these pollutants lead to a sig-
nificant boost in He-burning rates when a full nuclear reaction
network is utilized, allowing for nuclear reactions that bypass the
relatively slow triple-α process. Using the range of temperatures
and densities motivated in Section 3, we reexamine the issue of
He detonation ignition in more detail in Section 4. In addition
to constant density hotspots, we also consider constant pres-
sure hotspots that are more appropriate to the subsonic regions
where these detonations develop. We show in Section 4.3 that
these amendments to the previous calculations drastically de-
crease the minimum size of hotspots that give rise to He detona-
tions, making their realization in WD envelopes far more likely.

In Section 5, we calculate the propagation of these detonations
within He shells, allowing for post-shock radial expansion and
including the previously mentioned nucleosynthetic effects. We
find that propagating He detonations in the smallest allowable
shells yield 28Si and 40Ca as their main burning products, which
may explain the high-velocity features seen in many SNe Ia.

2. POLLUTED HELIUM-BURNING WITH A LARGE
NUCLEAR REACTION NETWORK

The majority of initial work on He detonations has as-
sumed initial compositions of pure He. However, as previ-
ously noted (e.g., Weinberg et al. 2006; Shen & Bildsten 2009;
Woosley & Kasen 2011), α-captures onto 12C and 16O seed
nuclei are far more rapid at the relevant temperatures than
the triple-α reaction, especially if the nuclear reaction net-
work used for the calculation includes the proton-catalyzed α-
capture 12C(p, γ)13N(α, p)16O. As mentioned previously, small
amounts of 12C and 16O are expected in the He-rich envelopes at
the time of detonation initiation. While the initial proton abun-
dance is likely very small, protons are also released in (α, p)
reactions involving the accreted 14N as well as α-chain nuclei
such as 20Ne, 24Mg, and 28Si.

Figure 1 shows He nuclei lifetimes versus temperature for
several direct and indirect α-capture reactions at a density of ρ =
107 g cm−3, where the lifetime is defined as |d ln Xα/dt|−1
due to reactions with the appropriate target isotope. The mass
fractions of He, 16C, 16O, and protons are Xα = 0.899, X12C =
X16O = 0.05, and Xp = 10−4. The lifetimes for the proton-
catalyzed reactions are calculated by assuming the intermediate
nuclei (13N and 17F) are in reaction rate equilibrium. It is
clear that pure α-captures onto 12C and 16O dominate over the
triple-α process for temperatures ≥109 K. Even more striking
is the reduction in the lifetime of He nuclei by four orders of
magnitude due to proton-catalyzed α-captures onto 12C seed
nuclei.

The inclusion of this reaction and the relevant isotopes and
reactions that enable it results in a dramatic boost in the He-
burning rate. Figures 2 and 3 show mass fractions (thick and
thin solid lines; see figures for the association of lines to
isotopes), temperature (dotted lines), and nuclear energy release
(dashed lines), q, as a function of time for two one-zone nuclear
burning calculations. In these one-zone burns, the density is held
constant at a value of 109 g cm−3, and the composition and
temperature are allowed to vary. The temperature thus obeys the
evolution equation

\[
\frac{dT}{dt} = \frac{\epsilon_{\text{nuc}} - \epsilon_{\nu}}{c_V},
\] (1)

![Figure 1](image1.png)

**Figure 1.** Lifetimes of He nuclei due to various nuclear reactions, as labeled, vs. temperature. The composition and density are given in the figure. (A color version of this figure is available in the online journal.)

![Figure 2](image2.png)

**Figure 2.** Mass fractions (solid lines), temperature (dotted line), and nuclear energy released (dashed line) vs. time. The initial composition is pure He, and the approximate nuclear reaction network is utilized. Apart from He, which is the black solid line that begins at Xα = 1, the solid lines, from left to right in order of their first appearance in time above a value of 10−3, represent 12C, 28Si, 32S, 38Ar, 40Ca, 44Ti, 48Cr, and 56Ni. The mass fractions of 16O, 20Ne, 24Mg, and 56Ni do not attain values ≥10−3. (A color version of this figure is available in the online journal.)
where the nuclear energy generation rate, $\epsilon_{\text{nuc}}$, the neutrino cooling rate, $\epsilon_\nu$, and the specific heat at constant volume, $c_V$, all depend on the changing composition and temperature.

The initial composition in Figure 2 is pure He, the initial composition in Figure 3 is $X_{\text{He}} = 0.891$, $X_{\text{C}} = X_{\text{O}} = 0.05$, and $X_{\text{N}} = 0.009$, and the initial temperature for both figures is $10^9$ K. The calculations here and throughout the rest of this paper utilize modules included with the MESA\(^4\) stellar evolution code (Paxton et al. 2011, 2013) for the implicit Rosenbrock integrator (Hairer & Wanner 1996), nuclear reaction rates (Cyburt et al. 2010), neutrino cooling rates (Itoh et al. 1996), and the equation of state (Timmes & Swesty 2000).

The nuclear burning network in Figure 2 is an often-used 13 isotope network, “aprox13” (Timmes 1999), which includes the 13 α-chain isotopes, forward and reverse α-captures, and $(\alpha, p)$($p, \gamma$) forward and reverse reactions for isotopes $^{24}\text{Mg}$ and heavier. In order to allow for $(p, \gamma)\alpha(p, \gamma)$ reactions at lower mass numbers, and any other possibly important reactions, the calculation shown in Figure 3 utilizes a 206 isotope nuclear network that tracks the abundances of neutrons, $^1\text{H}$, $^3\text{He}$, $^6\text{Li}$, $^7\text{Be}$, $^8\text{B}$, $^9\text{Be}$, $^{11}\text{B}$, $^{12}\text{C}$, $^{13}\text{N}$, $^{14}\text{O}$, $^{17}\text{F}$, $^{18}\text{O}$, $^{19}\text{F}$, $^{20}\text{Ne}$, $^{21}\text{Na}$, $^{22}\text{Mg}$, $^{23}\text{Al}$, $^{24}\text{Mg}$, $^{25}\text{Ca}$, $^{26}\text{Mg}$, $^{27}\text{Si}$, $^{28}\text{Si}$, $^{29}\text{P}$, $^{30}\text{Ar}$, $^{31}\text{Ar}$, $^{32}\text{Ar}$, $^{33}\text{Cl}$, $^{34}\text{Cl}$, $^{35}\text{Cl}$, $^{36}\text{Cl}$, $^{37}\text{K}$, $^{38}\text{Ca}$, $^{39}\text{Ca}$, $^{40}\text{Ca}$, $^{41}\text{Sc}$, $^{42}\text{Sc}$, $^{43}\text{Ti}$, $^{44}\text{Ti}$, $^{45}\text{Ti}$, $^{46}\text{Ti}$, $^{47}\text{Ti}$, $^{48}\text{Ti}$, $^{49}\text{Ti}$, $^{50}\text{Ti}$, $^{51}\text{V}$, $^{52}\text{V}$, $^{53}\text{V}$, $^{54}\text{Cr}$, $^{55}\text{Cr}$, $^{56}\text{Cr}$, $^{57}\text{Cr}$, $^{58}\text{Cr}$, $^{59}\text{Cr}$, $^{60}\text{Cr}$, $^{61}\text{Cr}$, $^{62}\text{Ni}$, $^{63}\text{Ni}$, $^{64}\text{Ni}$, $^{65}\text{Ni}$, $^{66}\text{Ni}$, $^{67}\text{Ni}$, $^{68}\text{Ni}$, $^{69}\text{Ni}$, $^{70}\text{Ni}$, and all of their interlinking nuclear reactions.

It is evident from a comparison of the two figures that the addition of a small amount of CNO isotopes and the use of a large reaction network vastly shortens the time to release a significant amount of energy. The polluted full network calculation reaches $q = 2 \times 10^{17}$ erg g$^{-1}$ more than 100 times faster than the pure He aprox13 case.\(^4\)

**Figure 3.** Same as Figure 2, but with a 206 isotope nuclear network and an initial composition of $X_{\text{He}} = 0.891$, $X_{\text{C}} = X_{\text{O}} = 0.05$, and $X_{\text{N}} = 0.009$. The black solid line beginning near a value of 1 represents the mass fraction of He, and the two solid lines beginning at 0.05 are $^{13}\text{C}$, which is depleted first, and $^{12}\text{C}$. The other solid lines represent the remaining α-chain isotopes in ascending mass order from their first appearance in time above a value of $10^{-3}$. The electron fraction remains essentially unchanged during the calculation from its initial value of 0.5. Note that non-α-chain isotopes are not displayed, even though some attain values $>10^{-3}$ during the course of the calculation. (A color version of this figure is available in the online journal.)

This speeding up of the energy release is demonstrated in Figure 4, which compares the results of four combinations of nuclear reaction networks and initial compositions. Two of the lines (“Pure He, aprox13” and “HeCNO, 206iso”) are as in Figures 2 and 3, respectively. The “Pure He, 206iso” calculation begins with an initial composition of pure He and utilizes the same 206 isotope network as in Figure 3. The “HeCNO, aprox13” calculation uses the aprox13 network and a polluted initial composition that mimics that of Figure 3, but the calculation shown in Figure 3 utilizes a 206 isotope nuclear network that tracks the abundances of neutrons, $^{1}\text{H}$, $^{3}\text{He}$, $^{6}\text{Li}$, $^{7}\text{Be}$, $^{8}\text{B}$, $^{9}\text{Be}$, $^{11}\text{B}$, $^{12}\text{C}$, $^{13}\text{N}$, $^{14}\text{O}$, $^{17}\text{F}$, $^{18}\text{O}$, $^{19}\text{F}$, $^{20}\text{Ne}$, $^{21}\text{Na}$, $^{22}\text{Mg}$, $^{23}\text{Al}$, $^{24}\text{Mg}$, $^{25}\text{Ca}$, $^{26}\text{Mg}$, $^{27}\text{Si}$, $^{28}\text{Si}$, $^{29}\text{P}$, $^{30}\text{Ar}$, $^{31}\text{Ar}$, $^{32}\text{Ar}$, $^{33}\text{Cl}$, $^{34}\text{Cl}$, $^{35}\text{Cl}$, $^{36}\text{Cl}$, $^{37}\text{K}$, $^{38}\text{Ca}$, $^{39}\text{Ca}$, $^{40}\text{Ca}$, $^{41}\text{Sc}$, $^{42}\text{Sc}$, $^{43}\text{Ti}$, $^{44}\text{Ti}$, $^{45}\text{Ti}$, $^{46}\text{Ti}$, $^{47}\text{Ti}$, $^{48}\text{Ti}$, $^{49}\text{Ti}$, $^{50}\text{Ti}$, $^{51}\text{V}$, $^{52}\text{V}$, $^{53}\text{V}$, $^{54}\text{Cr}$, $^{55}\text{Cr}$, $^{56}\text{Cr}$, $^{57}\text{Cr}$, $^{58}\text{Cr}$, $^{59}\text{Cr}$, $^{60}\text{Cr}$, $^{61}\text{Cr}$, $^{62}\text{Ni}$, $^{63}\text{Ni}$, $^{64}\text{Ni}$, $^{65}\text{Ni}$, $^{66}\text{Ni}$, $^{67}\text{Ni}$, $^{68}\text{Ni}$, $^{69}\text{Ni}$, $^{70}\text{Ni}$, and all of their interlinking nuclear reactions.

3. EXPECTATIONS FOR HOTSPOT CONDITIONS

Before exploring the effects of these decreased He-burning timescales on the initiation and propagation of detonations, we first estimate the characteristics of hotspots created during double WD mergers and during convective shell burning on WD surfaces to motivate the range of hotspot conditions we consider in Section 4.

### 3.1. Convective Hotspots

He detonations may arise in convective He-burning shells as they approach the point of inefficient convection, when the eddy turnover timescale becomes comparable to the local burning timescale, and the assumption of a globally isentropic envelope breaks down (Shen et al. 2010). We estimate the spectrum of temperature fluctuations in a convective shell by utilizing similar arguments to those employed for the situation of convective C-burning in WD cores (e.g., Woosley 2007; Pan et al. 2008; Schmidt et al. 2010).

We assume that the probability density function of turbulent energy dissipation fluctuations in the convective zone follows a

\(^4\) http://mesa.sourceforge.net, version 5596
log-normal distribution (Kolmogorov 1941, 1962):

$$pdf \left[ \ln \left( \frac{\epsilon_i}{\epsilon_H} \right) \right] = \frac{1}{\sqrt{2\pi} \sigma_l^2} \exp \left[ -\frac{\left( \ln \left( \frac{\epsilon_i}{\epsilon_H} \right) + \sigma_l^2/2 \right)^2}{2\sigma_l^2} \right],$$  \hspace{1cm} (2)

where $\sigma_l^2 \approx 0.2 \ln \left( H/l \right)$ (Schmidt et al. 2010), the integral scale height of the convective zone is $H$, and $l$ is the inertial length scale of interest. The mean energy dissipation rate at the largest scale is $\epsilon_H = v_{\text{conv}}^3/H$, where the convective velocity at the integral scale height is $v_{\text{conv}}$. Turbulent velocities at inertial length scales are $v_l = v_{\text{conv}}(l/H)^{1/2}$. The probability distribution function is normalized such that

$$\int_{-\infty}^{\infty} pdf \left[ \ln \left( \frac{\epsilon_i}{\epsilon_H} \right) \right] d \ln \left( \frac{\epsilon_i}{\epsilon_H} \right) = 1.$$  \hspace{1cm} (3)

The probability of obtaining a fluctuation $\epsilon < \epsilon_{\text{fluc}}$ is then

$$P(\epsilon < \epsilon_{\text{fluc}}) = \frac{1}{2} + \frac{1}{2} \text{erf} \left[ \frac{\ln \left( \frac{\epsilon_{\text{fluc}}}{\epsilon_H} \right) + \sigma_l^2/2}{\sqrt{2}\sigma_l^2} \right].$$  \hspace{1cm} (4)

The log-normal probability density function is not a complete description of intermittent turbulence (She & Lévéque 1994; Pan et al. 2008; Schmidt et al. 2010), but we utilize it here for simplicity and defer a more careful analysis to future work.

We wish to know the scale of the maximum dissipation fluctuation expected at a given length scale within the convective zone, $\epsilon_{\text{max}}(l)$. We estimate this by calculating the probability that none of the eddies with length scale, $l$, has a fluctuation larger than $\epsilon_{\text{max}}(l)$, and setting this probability equal to 50%. Within the volume of the convective zone, there are

$$N_l = \frac{4\pi R^2 l^3}{4\pi l^{1/3}} = \frac{3R^2}{H^2} \left( \frac{H}{l} \right)^3$$  \hspace{1cm} (5)

eddies of size $l$, where $R$ is the WD’s radius. Furthermore, the turbulent cascade at the length scale, $l$, is reset every local eddy turnover timescale, $\tau_l = 1/v_l$. There are then $N_l$ new instantiations during the global eddy turnover timescales, $\tau_{\text{global}} = H/v_{\text{conv}}$, where

$$N_l = \frac{\tau_{\text{global}}}{\tau_l} = \frac{H/v_{\text{conv}}}{1/v_l} = \left( \frac{H}{l} \right)^{2/3}. \hspace{1cm} (6)$$

Thus, $\epsilon_{\text{max}}(l)$ is implicitly given by

$$\frac{1}{2} = \left( \frac{1}{2} + \frac{1}{2} \text{erf} \left[ \frac{\ln \left( \frac{\epsilon_{\text{max}}(l)/\epsilon_H}{\epsilon_{\text{fluc}}/\epsilon_H} \right) + \sigma_l^2/2}{\sqrt{2}\sigma_l^2} \right] \right)^{N_l/N_0}.$$  \hspace{1cm} (7)

Since the fluctuation only acts over the local eddy turnover timescale before the distribution of eddies is reset, the increase in internal energy from this maximum fluctuation is given by

$$\delta \epsilon_{\text{max}}(l) = (\epsilon_{\text{max}}(l) - \epsilon_H) \tau_l = (\epsilon_{\text{max}}(l)/\epsilon_H - 1) v_{\text{conv}}^3 \left( \frac{l}{H} \right)^{2/3}. \hspace{1cm} (8)$$

The resulting expected maximum fluctuations and internal energy changes versus length scale are shown in Table 1 for typical values of the convective scale height of $10^8$ cm and a radius of $5 \times 10^8$ cm (suitable for a 0.05 $M_\odot$ envelope on a 1 $M_\odot$ WD as it approaches inefficient convection; Shen & Bildsten 2009). The $\delta \epsilon_{\text{max}}$ values, which scale directly with $v_{\text{conv}}^3$, assume $v_{\text{conv}} = 10^5$ cm s$^{-1}$. Typical values of the integral convective velocity range from 1–2 $\times 10^6$ cm s$^{-1}$.

| $l/H$ | $\epsilon_{\text{max}}(l)/\epsilon_H$ | $\delta \epsilon_{\text{conv}}/10^8$ erg g$^{-1}$ |
|------|----------------|------------------|
| 0.003 | 850 | 17 $\times 10^6$ |
| 0.01 | 230 | 11 $\times 10^6$ |
| 0.03 | 68 | 6.5 $\times 10^6$ |
| 0.1 | 18 | 3.7 $\times 10^6$ |
| 0.3 | 5.4 | 2.0 $\times 10^6$. |
of detonations occurs by a suitable gradient of induction time within a perturbed region, which is due to spatially varying fuel concentrations or thermodynamic variables. We consider hotspots with initially uniform composition and varying temperature and density gradients in this work; we defer a study of the effects of a spatially inhomogeneous composition to future research.

4.1. Description of Calculation

We take the temperature profiles within the hotspots to be linear in radius, so that

\[
T(r) = T_{\text{center}} - (T_{\text{center}} - T_0)\frac{r}{l_{\text{hotspot}}},
\]

where \(T_{\text{center}}\) is the temperature at the center of the hotspot, \(T_0\) is the temperature of the surrounding unperturbed medium, \(r\) is the distance from the hotspot’s center, and \(l_{\text{hotspot}}\) is the size of the perturbed region. Different parameterizations of the thermal profile will lead to somewhat different results; e.g., Seitenzahl et al. (2009) found that using linear, Gaussian, and exponential profiles changes the minimum detonatable size for C/O mixtures by a factor of a few. Since we only seek an estimate of the critical hotspot sizes, we defer the exploration of different profiles to future work. The surrounding temperature is taken to be \(10^7\) K for our calculations of detonation initiation. Calculations were also performed with \(T_0 = 10^8\) K, but the resulting minimum hotspot sizes are only altered by tens of percent, so we limit our results to \(T_0 = 10^7\) K.

We consider two types of density profiles: isochoric, or constant density, and isobaric, or constant pressure. The first is simply a constant density profile: the temperature is the only spatially varying quantity within the hotspot. For the isobaric case, the density profile varies in such a way as to keep the pressure spatially constant inside and outside the hotspot.

Previous studies have focused on isochoric hotspots. For densities and temperatures typical of C-burning calculations (Arnett & Livne 1994; Niemeyer & Woosley 1997; Röpke et al. 2007; Seitenzahl et al. 2009), isochoric hotspots are nearly isobaric because the hotspots are mostly electron degenerate, and thus the distinction is not very meaningful. However, for the lower-density conditions suitable for He-burning, the difference can be quite significant. An isobaric hotspot with a central temperature \(T_{\text{center}} = 10^9\) K and \(\rho_{\text{center}} = 10^5\) g cm\(^{-3}\) and a surrounding temperature of \(T_0 = 10^7\) K will have a surrounding density of \(\rho_0 = 5.0 \times 10^2\) g cm\(^{-3}\). This reduces the burning length scale (often referred to as the Zel’dovich—von Neumann—Döring, or ZND, length scale) in the surrounding medium by a large factor, which has important implications for minimum hotspot sizes. We will return to this point in the following sections.

As a result of the induction time gradient, the center of the hotspot burns first, followed by the surrounding region, and so on. This yields a burning front with an outward velocity equal to the inverse of the induction time gradient, \(v_{\text{burn}} = (dt_{\text{induction}}/dr)^{-1}\). For a detonation to develop, this burning front velocity should equal the steady-state detonation velocity (hereafter referred to as the Chapman—Jouguet, or CJ, velocity) at a point where at least a ZND length scale’s worth of material has been burned (Zel’dovich et al. 1970; He & Clavin 1994).

Our estimate of the minimum size of a hotspot that can transition to a detonation via the Zel’dovich gradient mechanism proceeds in the following way.

1. Specify the nuclear network, composition, central temperature and density of the hotspot, density profile (isochoric or isobaric), and surrounding temperature.
2. Calculate the surrounding density and the density profile within the hotspot if the hotspot is isobaric, assuming a linear temperature profile.
3. Choose a value for \(q\), the energy release of the propagating detonation.
4. Calculate the time to release this \(q\) at various points within the hotspot using one-zone burns as in Section 2. These induction times should be sampled densely enough within the hotspot such that they can be used to reliably calculate the induction time gradient. The induction times are calculated at a fixed density but changing temperature and composition. This mimics the formation of a supersonic burning front, for which the fluid elements do not have the necessary time to expand and change their density. Allowing for a changing composition is crucial for the production of trace isotopes (e.g., protons) that dramatically alter burning rates in large nuclear networks at high temperatures.
5. Calculate the CJ velocity and the ZND length scale in the surrounding unperturbed medium for a detonation that releases an energy equal to \(q\). These are estimated by starting with the post-shock, but pre-burned, material and following its time-dependent evolution at constant density. Here, the assumption of a constant density is not quite correct, as the density does change in a ZND calculation, but given the desired accuracy of our estimates, we do not consider this evolution.
6. Find the size of the hotspot such that the burning wave velocity equals the CJ velocity at a radius where a ZND length scale’s worth of material has already burned behind it.
7. Repeat for various values of \(q\) until the overall minimum detonatable hotspot size is found for the particular initial conditions specified in step 1.

The radius in step 6 is usually just where \(r = l_{\text{ZND}}\). However, because the triple-\(\alpha\) reaction rate decreases with increasing temperature \(\gtrsim 1.5 \times 10^9\) K, pure He hotspots with high maximum temperatures will not burn most rapidly near the center. This is especially true for isobaric hotspots where the density decreases toward the center, further increasing the induction time there. For these situations, we declare a successful detonation initiation if the burning velocity reaches the CJ value at a radius that is \(l_{\text{ZND}}\) outside of the point of minimum induction time.

4.2. Example Calculation

In this section, we demonstrate the process of determining the minimum detonatable hotspot for an isobaric pure He hotspot with a central temperature and density of \(T_{\text{center}} = 10^9\) K and \(\rho_{\text{center}} = 10^5\) g cm\(^{-3}\), a surrounding temperature of \(T_0 = 10^7\) K, and the approx13 nuclear network (Timmes 1999). Figure 5 shows the temperature and density profiles within the isobaric hotspot and surrounding unperturbed medium. The temperature profile is linear between the maximum temperature of \(10^9\) K at the center and the unperturbed value of \(10^7\) K at the edge of the hotspot. The density, which is \(10^5\) g cm\(^{-3}\) at the center, increases to a value of \(5.0 \times 10^5\) cm s\(^{-1}\) at the hotspot’s edge to keep the pressure constant.

\[\text{5 A similar acceleration due to the increasing temperature can be accounted for by the Frank–Kamenetskii factor (e.g., Khokhlov 1989), but an analogous factor accounting for the composition is difficult to define.}\]
The time evolution of the various points is calculated with the aprox13 network at a constant density and changing temperature and composition. The initial composition is pure He.

Since the temperature decreases outward while the density increases, the induction time does not monotonically increase with radius. This can be seen in Figure 6, which shows the time to release various values of $q$, as labeled, for the temperature and density profiles in Figure 5. The minima in induction times are at a radius roughly halfway between the center and the edge of the hotspot. As mentioned previously, the induction time is found by doing a time-dependent integration of the material at a constant density to simulate the formation of a supersonic wave.

The next step is to calculate the detonation properties in the unperturbed medium. The velocity of a steady-state planar detonation is given by the Chapman–Jouguet value of $v_{\text{CJ}} = \sqrt{2(\gamma^2-1)q}$, where $\gamma$ is assumed to be the value of both adiabatic indices, $\Gamma_1 = d \ln P / d \ln \rho|_s$ and $\Gamma_3 = 1 + d \ln T / d \ln \rho|_s$.

4.3. Results

We now show the results of our Zel’dovich gradient mechanism estimates for minimum detonatable hotspot sizes in He mixtures. Figure 8 shows minimum sizes as a function of the central temperature for constant density hotspots at three labeled densities. Dashed lines show our estimates for pure He media and the aprox13 network. Bullets show the numerical hydrodynamics results of Holcomb et al. (2013) for comparison. While the agreement between our results and theirs is not perfect, it is typically within tens of percent, giving us confidence that we are capturing the basic physics of the detonation initiation mechanism.

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

In practice, the values of $\Gamma_1$ and $\Gamma_3$ returned by the Helmholtz equation of state (Timmes & Swesty 2000) are slightly different, so an average of the two is used for $\gamma$.

For a given $v_{\text{CJ}}$, the standard shock jump conditions yield the temperature and density of the shocked but unburned material. Since the value of $\gamma$ depends on the post-shock temperature and density, we vary the CJ velocity until the derived $\gamma$ is self-consistent. The post-shock but pre-burn temperature and density are then used to perform a time-dependent integration at a constant density but changing temperature and composition. In a proper ZND calculation, the density also changes, but, for the sake of simplicity, we hold it constant.

This calculation yields the induction time of this material to release the assumed $q$. Multiplying this time by the CJ velocity yields an estimate of $l_{\text{ZND}}$, both of which are shown in Figure 7. The calculations are now in place for an estimate of the minimum detonatable hotspot size. For a given $q$, Figure 7 gives the CJ velocity and detonation length scale in the unperturbed medium. The size of the hotspot in Figure 6 is then adjusted until the burning wave velocity is equal to the CJ velocity at a distance that is a detonation length scale outside of the point of minimum induction time. The calculation is then repeated for various values of $q$ until a minimum detonatable hotspot size is found, which, for this fiducial example, is $8.3 \times 10^7$ cm at $q = 2.5 \times 10^{17}$ erg g$^{-1}$.

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

Figure 5. Density and temperature profiles for an isobaric hotspot with a linear temperature profile, $T_{\text{center}} = 10^8$ K, $\rho_{\text{center}} = 10^9$ g cm$^{-3}$, and $T_0 = 10^7$ K. The unperturbed density is $\rho_0 = 5.0 \times 10^5$ g cm$^{-3}$.

Figure 6. Induction time to release various values of $q$, as labeled, in the hotspot described in Figure 5. The time evolution of the various points is calculated with the aprox13 network at a constant density and changing temperature and composition. The initial composition is pure He.

Figure 7. ZND length scale and CJ velocity vs. $q$ in a medium with $T_0 = 10^7$ K and $\rho_0 = 5.0 \times 10^5$ g cm$^{-3}$. The initial composition is pure He, and the aprox13 nuclear network is utilized.
of composition was motivated by having one He nucleus for 9 but is significantly less than the pure He—aprox13 result of Holcomb et al. (2013). Dashed lines show our results for an initially pure He—aprox13 calculations of the structure of steady-state detonations need to be modified to account for the finite-gravity environment of the He envelope. Multidimensional simulations (Sim et al. 2012; Townsley et al. 2012; Moll & Woosley 2013) find steady He detonation velocities lower than the CJ velocity expected from fully burned one-dimensional calculations, mainly due to the quenching effects of the curvature of the detonation front as well as post-shock radial expansion.

Moore et al. (2013) investigated one-dimensional models of these effects, finding that there was a minimum He envelope mass that would support a steady detonation. Detonations in envelopes that were too small would experience significant quenching before a post-shock sonic locus was reached, preventing a self-sustaining detonation from forming. For envelopes large enough to support laterally propagating detonations, there is a one-to-one mapping between ambient conditions of an envelope (density, temperature, scale height, and composition) and a steady-state detonation solution. This allows us to identify an envelope structure with a single detonation length scale, \( l_{\text{ZND}} \) (here defined to be the length scale to 95% of the total energy release), and final-state nucleosynthesis. This final-state nucleosynthesis shows a strong dependence on envelope mass, with less massive envelopes producing mostly intermediate-mass elements described, the increased ambient density yields a smaller ZND length scale, which in turn leads to much smaller detonatable hotspot sizes. The pure He—aprox13 isobaric results approach the polluted—206 isotope isochoric results, and the polluted—206 isotope isobaric results are as much as 3000 times smaller than the pure He—aprox13 isochoric results. Our fiducial calculation at \( T_{\text{center}} = 10^9 \) K and \( \rho_{\text{center}} = 10^5 \) g cm\(^{-3}\) now results in a detonation for a 3 \( \times 10^6 \) cm hotspot, which is only 1% the WD’s scale height. This bodes extremely well for the possibility of igniting He detonations during shell convection or during WD mergers.

5. LATERAL PROPAGATION OF THE DETONATION

Now we investigate the steady-state structure of the laterally propagating surface detonation. Standard one-dimensional calculations of the structure of steady-state detonations need to be modified to account for the finite-gravity environment of the He envelope. Multidimensional simulations (Sim et al. 2012; Townsley et al. 2012; Moll & Woosley 2013) find steady He detonation velocities lower than the CJ velocity expected from fully burned one-dimensional calculations, mainly due to the quenching effects of the curvature of the detonation front as well as post-shock radial expansion.

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and significant 56Ni production only for high-mass envelopes where the quenching effects act on timescales long enough to allow for significant burning to occur. In this section, we present calculations with an improved version of the code from Moore et al. (2013), using the 206 isotope nuclear reaction network described in the previous sections.

Figure 10 shows how the minimum envelope mass that supports a steady detonation depends on the WD core mass, \( M_\text{env} \), for several reaction network and composition combinations. From top to bottom, the solid lines represent models with initial compositions of pure He and the approx13 nuclear network (blue), pure He and a 206 isotope network (orange), a polluted composition of \( X_{\text{He}} = 0.9 \) and \( X_{12C} = X_{16O} = 0.05 \) with the approx13 network (cyan), and a composition of \( X_{\text{He}} = 0.891, X_{12C} = X_{16O} = 0.05 \), and \( X_{14N} = 0.009 \) with 206 isotopes (black). The minimum shell masses where a significant portion of the ashes produced are radioactive on relevant timescales, (\( X_{\text{HeCNO}} + X_{52Cr} + X_{56Ni} > 0.2 \)) are shown as dotted lines for the same reaction networks and compositions. From top to bottom, the lines represent calculations with initially pure He and 206 isotopes (cyan), polluted He and 206 isotopes (black), pure He and approx13 (blue), and polluted He and approx13 (orange).

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Figure 11. ZND length scales (dashed line—right axis) and final mass fractions (solid lines—left axis) of material burned by a steady, laterally propagating detonation wave as a function of He envelope mass, \( M_{\text{env}} \), on a 1.0 \( M_\odot \) C/O WD. Each envelope mass corresponds to a unique detonation velocity eigenvalue and final-state composition. He is the most abundant element for the minimum-mass envelopes, followed by 28Si. The remaining solid lines, from left to right in order of their first appearance above \( X_i = 10^{-4} \), represent the mass fractions of 40Ca, 44Ti, 48Cr, 52Fe, and 56Ni. Non-\( \alpha \)-chain isotopes are not shown. (A color version of this figure is available in the online journal.)

Figure 10. Minimum envelope masses, \( M_{\text{env}} \), that can support a steady detonation as a function of WD core mass, \( M_\odot \), are shown in solid lines for several reaction network and composition combinations. From top to bottom, the solid lines represent models with initial compositions of pure He and the approx13 nuclear network (blue), pure He and a 206 isotope network (orange), a polluted composition of \( X_{\text{He}} = 0.9 \) and \( X_{12C} = X_{16O} = 0.05 \) with the approx13 network (cyan), and a composition of \( X_{\text{He}} = 0.891, X_{12C} = X_{16O} = 0.05 \), and \( X_{14N} = 0.009 \) with 206 isotopes (black). The minimum shell masses where a significant portion of the ashes produced are radioactive on relevant timescales, (\( X_{\text{HeCNO}} + X_{52Cr} + X_{56Ni} > 0.2 \)) are shown as dotted lines for the same reaction networks and compositions. From top to bottom, the lines represent calculations with initially pure He and 206 isotopes (cyan), polluted He and 206 isotopes (black), pure He and approx13 (blue), and polluted He and approx13 (orange).

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than the more realistic 206 isotope network. Additionally, varying the initial composition in the 206 isotope networks has little effect on the amount of radioactive isotopes produced in larger envelopes, despite allowing for successful detonations in smaller envelopes. The larger networks and more realistic compositions also increase the range of \( M_{\text{env}} \) where we expect little radioactivity in the burning products.

The use of the realistic composition and network allows for successful detonations in He-rich shells with masses \(<10^{-2} M_\odot \). This opens a new channel for double detonation SNe Ia in double C/O WD binaries, as C/O WDs are surrounded by thin He layers. While the accretors in these systems likely have very low-mass He envelopes \(<10^{-3} M_\odot \), donors \( \geq 0.6 M_\odot \) possess He layers \( \sim 10^{-2} M_\odot \), which may be enough to trigger a He detonation during the merging process. This possibility was first suggested by Raskin et al. (2012) and Pakmor et al. (2013), although neither global study could resolve the initiation and propagation of the detonation in the He layer surrounding the accreting WD. Future work on double detonation SNe Ia should allow for this channel, especially since there will be substantially more C/O pollution in the accreted He layer to further catalyze the detonation.

To get a picture of how the specific abundances are evolving as we vary the envelope mass, Figure 11 shows the sensitive dependence of the detonation products on the mass of the envelope for our fiducial polluted envelope composition on a 1.0 \( M_\odot \) WD core. Detonations in the lowest-mass envelopes are dominated by 28Si, 40Ca, and unburned He. Significant radioactivity requires higher-mass envelopes, with 56Ni only being produced by detonations in the most massive of envelopes. We define the detonation length scale, \( l_{\text{ZND}} \), as the post-shock distance to 95% of the total energy release. Since these are all pathological detonations, this typically occurs in the section of the post-shock flow that is supersonic relative to the detonation front, so not all of the energy produced can propel the detonation. As the envelope mass increases, the detonations get closer to the
limit of a Chapman–Jouget detonation, where all the burning occurs in material that is sonically connected to the detonation front. The qualitative behavior of such nucleosynthesis is the same for other WD core masses, with the minimum detonatable mass shifted depending on $M_d$.

The result that the minimum-mass detonatable shells produce intermediate-mass elements while avoiding iron-group element production is particularly interesting for double detonation SNe Ia from double WD binaries, as the He detonation will likely be triggered in the minimum-mass He shell. In merging systems, the ease of initiating the detonation may mean that the barrier to a successful detonation lies in the size of the shell, so that a fully propagating detonation is realized once the minimum He mass has been transferred from the donor. In stable mass transfer systems with a He donor, the accretion rate decreases from initially high values $M \sim 10^{-6} M_\odot \text{ yr}^{-1}$, and the system evolves from burning He stably to unsteadily. As $M$ decreases, the unstable He-burning events become more and more violent, until the size of the shell is large enough to support a propagating detonation. Thus, the first detonation in this stable mass transfer channel will also occur in the smallest detonatable shell.

If this minimum shell He detonation triggers a core detonation and a subsequent SN Ia, the He shell ashes will not yield large amounts of high-velocity iron-group elements, which have been ruled out by several studies (e.g., Nugent et al. 1997; Kromer et al. 2010). The minimum-mass shells will instead consist of high-velocity unburnt He, $^{28}\text{Si}$, $^{40}\text{Ca}$, and a small amount of unburnt primordial metals. Given the lack of non-thermal electrons, the He will likely stay neutral and unobservable. The remaining elements may explain observations of high-velocity absorption features seen in most SNe Ia (Mazzali et al. 2005; Tanaka et al. 2008; Blondin et al. 2012; Childress et al. 2014; Maguire et al. 2014). Further work is necessary to determine if the strong abundance enhancements of the $^{28}\text{Si}$, $^{40}\text{Ca}$, and other metals are enough to produce these features. However, given that they comprise essentially all of the opaque material at these velocities, this is a very promising avenue of future research.

6. CONCLUSIONS

In this paper, we have shown that the ignition of He detonations and their propagation in WD envelopes are significantly impacted by the inclusion of a small amount of C/O pollution and a full nuclear reaction network. Motivated by an examination of the relevant reaction rates in Section 2 and hotspot conditions in Section 3, our calculations in Sections 4 and 5 indicate that He detonation ignition and propagation is possible during double WD mergers and in convectively burning envelopes on WD surfaces and is thus a promising channel for SNe “Ia” and “Ia2.

Detonations in low-mass He envelopes may produce high-velocity Si, Ca, and unburned metal spectral features if a double detonation occurs and the core explodes as a SN Ia. If the He envelope detonates without triggering a secondary detonation in the WD core (either due to weak shock focusing or a core composition of O/Ne), then it could appear as a “Ia2” SN if significant radioactive isotopes are produced. Otherwise, the low ejecta mass coupled with little to no radioactivity in the ashes would produce a virtually unobservable explosion, perhaps detectable as circumstellar material if illuminated by subsequent explosions.

Given the relative infancy of work regarding He detonation ignition and propagation, it is clear that further study is required. Future work will include multidimensional hydrodynamic cal-

We thank Lars Bildsten, James Guillochon, Falk Herwig, Bill Paxton, Eliot Quataert, Ivo Seitenzahl, Frank Timmes, and Dean Townsley for helpful discussions and the referee for their comments. K.J.S. acknowledges the hospitality of Caskhouse, where some of these calculations were performed. K.J.S. is supported by NASA through the Astrophysics Theory Program (NNX15AB16G) and the Einstein Postdoctoral Fellowship (PF1-120088) awarded by the Chandra X-ray Center, which is operated by the Smithsonian Astrophysical Observatory for NASA under contract NAS8-03060. K.M. is partially supported by the National Science Foundation under grant AST 11-09174.

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