INCOMPLETE CARBON–OXYGEN DETONATION IN TYPE Ia SUPERNOVAE

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\begin{abstract}

Incomplete carbon–oxygen detonation with reactions terminating after burning of C\textsuperscript{12} in the leading C\textsuperscript{12} + C\textsuperscript{12} reaction (C-detonation) may occur in the low-density outer layers of white dwarfs exploding as Type Ia supernovae (SNe Ia). Previous studies of carbon–oxygen detonation structure and stability at low densities were performed under the assumption that the \textit{velocity} of a detonation wave is derived from complete burning of carbon and oxygen to iron. In fact, at densities $\rho \lesssim 10^6$ g cm$^{-3}$ the detonation in SNe Ia may release less than a half of the available nuclear energy. In this paper, we study basic properties of such detonations. We find that the length of an unsupported steady-state C-detonation is $\simeq 30$–100 times greater than previously estimated and that the decreased energy has a drastic effect on the detonation stability. In contrast to complete detonations which are one-dimensionally stable, C-detonations may be one-dimensionally unstable and propagate by periodically re-igniting themselves via spontaneous burning. The re-ignition period at $\rho \lesssim 10^6$ g cm$^{-3}$ is estimated to be greater than the timescale of an SN Ia explosion. This suggests that propagation and quenching of C-detonations at these densities could be affected by the instability. Potential observational implications of this effect are discussed.

\textit{Key words:} hydrodynamics – instabilities – nuclear reactions, nucleosynthesis, abundances – shock waves – supernovae: general – white dwarfs
\end{abstract}

1. INTRODUCTION

Type Ia supernovae (SNe Ia) are thermonuclear explosions of carbon–oxygen white dwarfs (CO-WDs) in binary stellar systems. Explosion models of SNe Ia currently discussed in the literature include explosions of Chandrasekhar-mass WDs, such as delayed detonation (DD), pulsating DD and its variants (Khokhlov 1991a, 1991b; Gamezo et al. 2005; Livne et al. 2004; Plewa et al. 2007; Livne et al. 2005; Röpke & Niemeyer 2007; Jordan et al. 2008; Meakin et al. 2009) and pulsating reverse detonations (Bravo & García-Senz 2006; Bravo et al. 2009; Bravo & García-Senz 2009), explosions of sub-Chandrasekhar WDs (Woosley et al. 1980; Nomoto 1982; Livne & Glasner 1991; Livne & Arnett 1995; Fink et al. 2007, 2010), and supermassive WDs (Pfannes et al. 2010). These models differ in their assumptions about initial conditions, ignition processes, whether the explosion involves subsonic deflagration or not, and other details, and they have a varying success in explaining basic observations of SNe Ia (this subject is outside of the scope of the paper). A common feature of the models is that all of them involve, in one way or another, the detonation mode of burning.

Detonation is a supersonic wave of burning in which reactions are triggered by a strong shock. The energy released by burning maintains the shock strength and propagation of the detonation wave. A steady-state detonation is described by the ZND theory (Zeldovich 1940; von Neumann 1942; Döring 1943) according to which the detonation wave consists of a leading planar shock followed by a one-dimensional reaction zone. A ZND detonation structure is usually unstable due to a strong positive feedback between hydrodynamical perturbations and energy release inside the reaction zone, and a real detonation propagates non-steadily with strong oscillations and transverse waves which form a multi-dimensional cellular structure of a detonation wave (e.g., Fickett & Davis 1979; Lee 1984; Shepherd 2009).

Explosive burning in an SN Ia consists of three distinct stages: burning of carbon to O, Ne, Na, Mg, and some Si (C-burning); subsequent burning of oxygen and formation of Si-group elements (O-burning); and finally burning of silicon to Fe-group elements (Si-burning). Nuclear statistical equilibrium (NSE) in burned matter sets in at the end of Si-burning. Timescales of C, O, and Si-burning, $t_C$, $t_O$, and $t_S$ differ by orders of magnitude, $t_C \ll t_O \ll t_S$, and increase exponentially with decreasing temperature. Due to the existence of three distinct stages of burning, a CO detonation wave in an SN Ia consists of C-, O-, and Si-burning layers of increasing thickness, $x_C \ll x_O \ll x_S$, following each other. All three thicknesses depend on density, $\rho$, and increase exponentially with decreasing $\rho$. The thickness of Si and O-burning layers, $x_S$ and $x_O$, becomes greater than the characteristic scale of an exploding WD ($\simeq 10^6$ cm) at $\rho \lesssim 10^7$ g cm$^{-3}$ and $\rho \lesssim 10^6$ g cm$^{-3}$, respectively (e.g., Khokhlov 1989; Gamezo et al. 1999; Sharpe 1999). Equivalently, it could be said that at these densities $t_S$ and $t_O$ become greater than the characteristic explosion timescale of a WD $\lesssim 1$ s. An important observational property of SNe Ia, as was inferred early from near-maximum spectra, is the presence of intermediate mass elements such as Si, S, Ca, Mg, Na, and O in the outer layers of an SN Ia envelope (e.g., Pskovskii 1969; Branch et al. 1982, 1983). The presence of these elements can be explained as a consequence of incomplete burning at low densities $\rho \lesssim 10^7$ g cm$^{-3}$.

Whether and how the instability and cellular structure of a detonation influence the explosion of an SN Ia have been long-standing questions. Time-dependent interplay of nuclear reactions and hydrodynamical motions in a detonation wave may affect explosive nucleosynthesis and quenching of burning. Incomplete C-burning may leave some carbon intact. This may be important for prediction of chemical composition and formation of light curves and spectra of SNe Ia before and near maximum light. Due to the resolution limitations, these effects were studied in idealized constant-density conditions representing small parts of an exploding WD. A one-dimensional longitudinal...
instability of CO detonations was studied numerically in Khokhlov (1993; see also Koldoba et al. 1994). Cellular structure of CO detonations was obtained in numerical simulations of Boisseau et al. (1996), Gamezo et al. (1999), and Timmes et al. (2000). Calculations show that cellular structure associated with O- and Si-burning might be potentially important and affect burning at densities $\rho \leq 10^2$ g cm$^{-3}$ but cellular structure related to C-burning appears to be very small at all densities of interest, say, at $\rho > 10^3$ g cm$^{-3}$.

For low-density detonations the simulations mentioned above contain a serious deficiency. The reason is as follows. The simulations use background conditions (density, temperature, etc.) and the detonation velocity as input parameters. These parameters are used to establish initial and boundary conditions for a simulation. The simulation then gives information about scales and stability of a detonation wave. In the above simulations, it was assumed that the input detonation velocity corresponds to a complete burning to NSE. For detonations at low density this leads to a contradiction: Si- and O-burning at low densities may not occur and a detonation wave may consist of a shock wave followed either by C- and O-burning layers (O-detonation) or by a C-burning layer alone (C-detonation). Nuclear energy released in such detonation waves will be smaller than the NSE energy release. It is this reduced energy release which must be used for calculating the input detonation velocity. The assumption of NSE will lead to a higher detonation velocity, overprediction of post-shock temperature and density, underestimation of a detonation wave thickness, and may affect detonation stability and propagation.

In this paper, we revisit the problem of detonation structure and stability taking into account the reduction of energy release in incomplete detonation waves. We try to answer the following questions: What are the basic properties and characteristic spatial and temporal scales of incomplete O- and C-detonation waves at low densities? How unstable are these detonations? What is the timescale of the instability and how does it compare to other scales of the problem? To what extent may the instability affect quenching of a detonation wave and the resulting nucleosynthesis? In this paper we study ZND structure and one-dimensional stability of incomplete detonations. Propagation of a detonation wave is also influenced by multi-dimensional effects but a one-dimensional investigation should be the first step. In this paper, we find that a C-detonation could be a factor of $\approx 30–100$ thicker than previously thought and that C-detonations could be highly unstable with respect to one-dimensional longitudinal perturbations. Multi-dimensional study of C-detonations will be presented in a following paper.

The paper is organized as follows. Section 2 presents the governing equations and input physics. Section 3 discusses the properties of steady-state detonations with complete and partial energy release. Section 4 describes the numerical simulations and presents the analysis of one-dimensional stability of the detonations. The results and potential implications for SN Ia modeling and observations are discussed in Section 5. The numerical method and test simulations are described in the Appendix.

2. FORMULATION OF THE PROBLEM

The propagation of a one-dimensional detonation wave is described by the time-dependent, compressible, reactive flow Euler equations of fluid dynamics:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial (\rho u)}{\partial x},$$

$$\frac{\partial \rho u}{\partial t} = -\frac{\partial (\rho u^2 + P)}{\partial x},$$

$$\frac{\partial E}{\partial t} = -\frac{\partial (u(E + P))}{\partial x} + \rho q,$$

$$\frac{\partial \rho \tilde{Y}}{\partial t} = -\frac{\partial (\rho \tilde{Y})}{\partial x} + \rho \tilde{R},$$

for mass density $\rho$, velocity $u$, energy density $E = \rho (\epsilon + \frac{\tilde{Y}}{\rho})$, where $\epsilon$ is internal energy per unit mass, and the composition of reactants $\tilde{Y} = \{Y_1, ..., Y_N\}$ defined as $Y_i = n_i/\rho N_a$, where $N$ is the number of reactants, $n_i$ are their number densities and $N_a$ is the Avogadro number. $\tilde{R} = \{R_1, ..., R_N\}$ are the corresponding net reaction rates which are functions of $\tilde{Y}$, $\rho$, and temperature $T$. The energy generation rate due to nuclear reactions is

$$\dot{q} = \tilde{Q} \cdot \tilde{R} = \sum_{i=1}^{N} Q_i R_i,$$

where $\tilde{Q} = \{Q_1, ..., Q_N\}$ are the binding energies of nuclei. The numerical method of integration of Equations (1)–(4) is described in the Appendix.

Nuclear kinetics is described by the $\alpha$-network which has been extensively used in previous studies of detonation stability and cellular structure (Khokhlov 1993; Gamezo et al. 1999; Timmes et al. 2000). The network consists of $N = 13$ nuclei He$^4$, C$^{12}$, O$^{16}$, Ne$^{20}$, Mg$^{24}$, Si$^{28}$, S$^{32}$, Ar$^{36}$, Ca$^{40}$, Ti$^{44}$, Cr$^{48}$, Fe$^{52}$, and Ni$^{56}$. The network takes into account binary reactions between $\alpha$-particles and heavier nuclei C$^{12} + \alpha \leftrightarrow$ O$^{16} + \gamma$, O$^{16} + \alpha \leftrightarrow$ Ne$^{20}$, ..., Fe$^{52} + \alpha \leftrightarrow$ Ni$^{56}$; C$^{12} +$ C$^{12} \leftrightarrow$ O$^{16}$ and O$^{16} +$ O$^{16}$ and a triple-alpha reaction $3\alpha \leftrightarrow$ C$^{12} + \gamma$. Effective reaction rates of binary reactions involving $\alpha$ particles are calculated as the sums of contributions of $(\alpha, p)(\gamma)$, $(\alpha, n)(n, \gamma)$, $(\alpha, \gamma)$ reaction channels involving $p$, $n$, and $\gamma$-photons. Forward reaction rates and partition functions are taken from compilations of Fowler et al. (1978), Woosley et al. (1978), and Thielemann et al. (1987). Reverse reaction rates are calculated from the principle of detailed balance. The network captures the multi-stage nature of explosive CO burning and correctly reproduces the timescales of C-, O-, Si-burning stages, and the onset of nuclear statistical quasi-equilibrium (NSQE) and NSE in nuclear matter. The equation of state includes contributions from ideal Fermi–Dirac electrons and positrons with arbitrary degeneracy and relativism, equilibrium Planck radiation, and ideal Boltzmann nuclei.

3. STEADY-STATE CO DETONATIONS

3.1. ZND Detonation in CO Mixtures

Steady-state detonation solutions provide basic temporal and spatial scales of a detonation wave and are also used as initial conditions for time-dependent numerical simulations. In a reference frame moving with detonation velocity, $D$, all variables inside a one-dimensional steady-state detonation wave are a function of the distance, $x$, from the leading shock and do not depend on $t$. We denote by subscripts $0$, $s$, and $d$ hydrodynamical variables in unburned cold matter, in unburned matter located immediately behind the leading shock, and in detonation products, respectively. Hydrodynamical variables inside the reaction zone are related to hydrodynamical variables in unburned matter through the Hugoniot relations:

$$\rho u = \rho_0 D.$$
possible detonation velocity, $D = D_{CJ}$. An unsupported detonation propagates in this regime if $q$ is a monotonic function of $x$. Overdriven detonations are possible in this case for all velocities $D > D_{CJ}$. This is the case for all detonations at $\rho_0 \leq 2 \times 10^7$ g cm$^{-3}$ considered in the paper. For higher densities the energy release in 0.5C + 0.5O detonations is not monotonic and an unsupported detonation propagates in a pathological regime with some velocity $D^* > D_{CJ}$. Overdriven detonations in this case are possible for $D > D^*$. For a few simulations of high-density detonations presented in this paper, we used as initial conditions slightly overdriven detonation solutions with $D$ very close to $D^*$. A detailed explanation of a pathological detonation can be found in Fickett & Davis (1979) and for CO detonations in Khokhlov (1989) and Sharpe (1999).

### 3.2. CO Detonations with Complete Energy Release

As mentioned in Section 1, explosive burning of CO mixtures proceeds through three consecutive stages: burning of C$^{12}$ in the leading C$^{12} +$ C$^{12}$ reaction, burning of O$^{16}$ and the formation of Si-group elements, and Si-burning which creates Fe-peak elements. The state of NSE is reached at the end of Si-burning. As a result, the detonation waves in carbon–oxygen have a multi-layered structure with C-burning, O-burning, and Si-burning layers with increasing thickness, $x_C \ll x_O \ll x_{Si}$, which follow each other. The CJ detonation structure for a 0.5C + 0.5O detonation at $\rho_0 = 3 \times 10^6$ g cm$^{-3}$ is shown in Figure 2 as an example. The distinct C-burning, O-burning, and Si-burning layers are clearly visible. C-burning releases $q_C \simeq 0.35$ MeV nucleon$^{-1}$ of nuclear energy, at the end of the O-burning the total released energy is $q_{O} \simeq 0.65$ MeV nucleon$^{-1}$, and the total energy released at the end of the reaction zone is $q_{NSE} \simeq 0.8$ MeV nucleon$^{-1}$. The detonation products at this density are mostly composed of Ni.

In what follows we will characterize detonations in CO mixtures with the overdrive parameter

$$f = \left( \frac{D}{D_{CJ,NSE}} \right)^2$$

calculated with respect to the CJ detonation velocity of the complete detonation in which burning proceeds to NSE. Pathological detonation occurring at $\rho_0 > 2 \times 10^7$ g cm$^{-3}$ has an overdrive $f^* = (D^*/D_{CJ,NSE})^2 > 1$. Calculations show that deviation of $f^*$ from 1 are relatively small. For $\rho_0 = 3 \times 10^6$ g cm$^{-3} f^* \simeq 1.01$. For higher densities $f^*$ increases to $f^* \simeq 1.07$. Figure 3 shows an overdriven detonation solution for $\rho_0 = 10^8$ g cm$^{-3}$ with $f = 1.08$ which is very close to the pathological regime at this density. Again, the distinct C-burning, O-burning, and Si-burning layers can be clearly seen. Similar to the previous case, C-burning releases $q_C \simeq 0.36$ MeV nucleon$^{-1}$ of nuclear energy but due to photodissociation of nuclei in the O-burning and Si-burning layers $q_O$ is reduced to $\simeq 0.5$ MeV nucleon$^{-1}$ and the overall detonation energy to $q_{NSE} \simeq 0.37$ MeV nucleon$^{-1}$, resulting in the non-monotonic energy release. For detonations with non-monotone energy release we find that maximum of $q$ occurs near the maximum of the concentration of Si. The energy release in the C-burning layer is always monotonic, so that C-detonation will always not be pathological.

Figure 4 gives $x_C, x_O$, and $x_{Si}$ for unsupported 0.5C + 0.5O detonations as a function of $\rho_0$; $x_C$ and $x_O$ are defined as half-reaction zone thickness where the concentrations of C$^{12}$ and
O\text{16} diminish to one-half of their initial values, respectively: \(x_{\text{Si}}\) is defined as a thickness where Si decreases to one-half of its maximum value inside the reaction zone. The total thickness of the detonation wave, \(x_{\text{NSE}}\), corresponds to 90 % of the Ni synthesized in the detonation wave. The horizontal dotted line in Figure 4 shows the characteristic size of an exploding WD, \(R_{\text{WD}} \approx 10^8 \text{ cm}\). For \(\rho < \rho_{\text{NSE}} \approx 10^7 \text{ g cm}^{-3}\), \(x_{\text{NSE}} \gg R_{\text{WD}}\) which means that burning in a detonation wave will not have time to reach the state of NSE. At \(\rho < \rho_{\text{Si}} \approx 5 \times 10^6 \text{ g cm}^{-3}\) the reaction zone of a CJ detonation will consist of the C-burning layer followed by the O-burning layer but the Si-layer will be absent. At \(\rho \lesssim \rho_{\text{CJ}} \approx 10^6 \text{ g cm}^{-3}\) \(x_{\text{O}} \gg R_{\text{WD}}\) and the reaction zone will consist of the C-burning layer alone.

### 3.3. Carbon Detonations with Reduced Energy Release

Due to the large separation between the reaction scales of C-, O-, and Si-burning, an incomplete detonation may be considered as an isolated C-detonation (or an O-detonation) wave with reduced energy release \(q_{\text{C}} \approx 0.35 \text{ MeV nucleon}^{-1}\) (or \(q_{\text{O}} \approx 0.65 \text{ MeV nucleon}^{-1}\) for O-detonation). At densities \(\rho < 10^6 \text{ g cm}^{-3}\) photodissociation of nuclei is insignificant and \(q_{\text{C}}\) and \(q_{\text{O}}\) are practically density-independent. For C-detonation the situation is schematically illustrated in Figure 1. The figure shows a C-detonation adiabat with energy release \(q_{\text{C}}\) or \(q_{\text{O}}\). The R-M line \(s^3\)-Cl\text{C}\ corresponds to a CJ C-detonation with velocity \(D_{\text{CJ,C}} < D_{\text{CJ,NSE}}\).

By analogy with (11) we can also characterize C-detonations with the overdrive parameter defined relative to \(D_{\text{CJ,C}}\).

\[
f_{\text{C}} = \left(\frac{D}{D_{\text{CJ,C}}}\right)^2 = f \cdot \left(\frac{D_{\text{CJ,NSE}}}{D_{\text{CJ,C}}}\right)^2 > f.
\]

Then C-burning layer of a CJ NSE detonation, segment \(s^1\)-c1 in Figure 1, can be viewed as a C-detonation overdriven to \(f_{\text{C}} = (D_{\text{CJ,NSE}}/D_{\text{CJ,C}})^2\). All C-detonations with velocities between \(D_{\text{CJ,C}}\) and \(D_{\text{CJ,NSE}}\), such as \(s^2\)-c2, can be considered as overdriven detonations with overdrive parameters \(1 < f_{\text{C}} < (D_{\text{CJ,NSE}}/D_{\text{CJ,C}})^2\). Equivalently, they are underdriven detonations characterized by \(f\) ranging from \((D_{\text{CJ,C}}/D_{\text{CJ,NSE}})^2\) to one. The same detonation can be characterized by using either \(f\) or \(f_{\text{C}}\) which are related by (12). In this paper, we choose to uniformly parameterize all detonations using \(f\). The above consideration equally applies to O-detonations with the replacement of \(q_{\text{C}}\) with \(q_{\text{O}}\) and \(D_{\text{CJ,C}}\) with the corresponding value of \(D_{\text{CJ,O}}\).

Since C- and O-detonations have lower energy release, their temporal and spatial scales are larger than those of the NSE detonations. Figure 5 shows the reaction zone length \(x_{\text{C}}\) and \(x_{\text{O}}\) for C-detonations and O-detonations as a function of \(f\) for densities \(\rho = 10^6, 3 \times 10^6, 10^7 \text{ g cm}^{-3}\). The curves begin on the left at the values of \(f\) which correspond to the CJ regimes of the C- and O-detonations. On the right, all curves terminate at \(f = 1\) where the C- and O-detonations become a part of a complete CJ NSE detonation moving with velocity \(D_{\text{CJ,NSE}}\).
Figure 3. Overdriven detonation structure for 0.5C + 0.5O mixture at \( \rho_0 = 10^8 \text{ g cm}^{-3} \) and \( f = 1.08 \). Top: pressure, middle: temperature in \( 10^9 \text{ K} \), bottom: mass fractions of nuclei (solid curves) and nuclear energy release (dashed line). Distance is normalized to a half-reaction length of a C-burning layer. The shock wave is on the left (at \(-\infty\) in logarithmic coordinates).

The spatial scales of the C- and O-detonations increase with decreasing \( f \) exponentially. For CJ C-detonation \( x_C \) exceeds the thickness of the \( f = 1 \) detonations by a factor \( \approx 30–100 \).

4. ONE-DIMENSIONAL PROPAGATION OF CO DETONATIONS

4.1. Detonation Stability

Numerical simulations of detonation propagation are listed in Table 1. Details of a numerical approach and test simulations are described in the Appendix. For each simulation the table gives the initial density \( \rho_0 \), the overdrive \( f \), and other parameters of a steady-state detonation. Column 7 of the table describes the non-steady behavior of a detonation wave found in the simulations: “S”—stable propagation, “O” and “D”—unstable propagation.

In O-type cases, we observed several cycles of oscillations of the detonation wave. In D-type cases the detonation rapidly decayed, the leading shock wave decoupled from the reaction zone, and the re-ignition of the detonation did not occur over the time of numerical integration. This does not mean that the detonation dies and never re-ignites but that the re-ignition does not occur on a timescale of at least \( \approx L/a_s \), where \( L \) is the length of the computational domain and \( a_s \) is the sound speed. The re-ignition time for D-type detonations is estimated in Section 4.3.

Figure 6 summarizes the stability properties of the calculated detonations in the \( \rho_0-f \) plane. The boundary of detonation
Detonations with densities $\rho_0 > 2 \times 10^7$ g cm$^{-3}$ at low densities the curve passes through overdriven regimes of C-detonations with $f < 1$. The stability curve crosses the $f = 1$ line at $\rho_0 = 2 \times 10^7$ g cm$^{-3}$.

It must be stressed that at all densities the regimes located at the stability curve are characterized by $f_C > 1$ and are overdriven with respect to the CJ C-detonation. The freely propagating C-detonations are highly unstable and exhibit the D-type behavior. Overdriven detonations with $f = 1.08$ calculated for high densities $\rho_0 \geq 10^9$ g cm$^{-3}$ have the structure of the C-burning layer which is very close to that of freely propagating pathological detonations. These detonations are highly unstable and exhibit D-type behavior as well.

Changes in the detonation behavior when $\rho_0$ is fixed and $f$ is decreasing are illustrated in Figure 7 for $\rho_0 = 3 \times 10^6$ g cm$^{-3}$. At this density the detonation with $f = 0.76$ is stable whereas the detonation with $f = 0.71$ is unstable, from which we may deduce that the boundary of stability at this density is located between these two values of $f$. The linear interpolation gives $f_c \approx 0.73$. The detonation with $f = 0.71$ is mildly unstable (Figure 7(a)). The initial slow growth of perturbations is followed by regular oscillations with a period $\Pi \approx 9.5\, \tau_C$ and an amplitude $\Delta \approx 0.1$ of the steady-state post-shock pressure. For the detonation with $f = 0.62$ the instability develops more rapidly. The quasi-periodic oscillations have a much larger amplitude $\Delta \approx 0.6$.

The quasi-periodic oscillations have a much larger amplitude $\Delta \approx 0.6$.

| $\rho_0$/10$^6$ | $f$ | $\rho_0$/10$^6$ | $f$ | $T/s$ | $D^\alpha$ | $\Theta^{-1}$ | $(\ln T/\ln\epsilon)_\rho$ | $\ln(\rho/\rho_0)$ | $\beta$ |
|-----------------|-----|-----------------|-----|--------|--------|-----------------|-----------------|------------------|--------|
| 1.0 $\times$ 10$^6$ | 1.00 | 4.80 | 24.3 | 3.85 | 1.21 | S | 19.6 | 0.43 | 0.65 | 6.14 |
| 1.00 | 1.00 | 4.80 | 24.3 | 3.85 | 1.21 | S | 19.6 | 0.43 | 0.65 | 6.14 |
| 0.79 | 4.84 | 30.5 | 2.81 | 1.04 | S | 20.4 | 0.52 | 0.77 | 8.21 |
| 0.71 | 4.69 | 27.3 | 2.65 | 0.98 | O | 20.8 | 0.57 | 0.86 | 10.1 |
| 0.58 | 4.43 | 22.2 | 2.35 | 0.89 | O | 21.7 | 0.67 | 1.03 | 15.0 |
| 0.55 | 4.35 | 21.0 | 2.27 | 0.87 | D | 21.9 | 0.70 | 1.08 | 16.6 |
| 2.0 $\times$ 10$^6$ | 1.00 | 4.80 | 24.3 | 3.85 | 1.21 | S | 19.6 | 0.43 | 0.65 | 6.14 |
| 1.00 | 1.00 | 4.80 | 24.3 | 3.85 | 1.21 | S | 19.6 | 0.43 | 0.65 | 6.14 |
| 0.77 | 4.47 | 19.1 | 3.35 | 1.07 | S | 19.2 | 0.51 | 0.76 | 8.37 |
| 0.71 | 4.33 | 17.1 | 3.12 | 1.02 | O | 19.7 | 0.79 | 0.74 | 11.4 |
| 0.62 | 4.13 | 15.0 | 2.86 | 0.96 | O | 20.3 | 0.88 | 0.82 | 14.6 |
| 0.58 | 4.03 | 14.0 | 2.72 | 0.92 | D | 20.6 | 0.94 | 0.87 | 16.8 |
| 0.55 | 3.97 | 13.2 | 2.60 | 0.90 | D | 20.9 | 0.99 | 0.91 | 18.9 |
| 3.0 $\times$ 10$^6$ | 1.02 | 3.57 | 8.20 | 4.39 | 1.16 | O | 17.6 | 0.63 | 0.43 | 12.4 |
| 0.94 | 3.45 | 7.64 | 4.12 | 1.13 | O | 18.0 | 0.78 | 0.45 | 14.4 |
| 0.94 | 3.42 | 7.49 | 4.04 | 1.12 | D | 18.1 | 0.86 | 0.46 | 15.1 |
| 1.0 $\times$ 10$^7$ | 1.08 | 2.95 | 5.30 | 4.36 | 1.19 | D | 17.6 | 3.10 | 0.36 | 19.6 |
| 3.0 $\times$ 10$^7$ | 1.08 | 2.94 | 3.82 | 4.16 | 1.23 | D | 17.9 | 6.00 | 0.32 | 34.4 |

Notes.

a $\rho_0$ is in g cm$^{-3}$; $T_0$ is in 10$^9$ K; $D$ is in 10$^5$ cm s$^{-1}$.

b Detonations with $f \geq 1$ are calculated assuming NSE in products of burning (Section 3.2). Detonations with $f < 1$ are C-detonations (Section 3.3).

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Figure 5. Thickness of C-detonation ($x_C$, solid lines) and O-detonation ($x_O$, dashed lines) as a function of overdrive $f \leq 1$ for densities $\lg(\rho_0) = 6.0, 6.5, 7.0, \rho_0$ is in g cm$^{-3}$.
Figure 6. Summary of calculations of time-dependent propagation in $0.5C + 0.5O$ mixtures. Open circles: stable detonations; open triangles: unstable oscillating detonations; solid triangles: unstable detonations for which the oscillation cycle was not calculated. Solid line: the estimated stability curve. Dashed line: timescale of the oscillation cycle exceeds $\simeq 200t_C$ where $t_C$ is the half-reaction timescale of a steady-state C-detonation. Dash-dotted line: location of Chapman–Jouguet detonations, $f = 1$.

Figure 7. Post-shock pressure $P_s(t)$ for C-detonations with different overdrives at $\rho_0 = 3 \times 10^6$ g cm$^{-3}$. (a) $f = 0.71$, (b) $f = 0.62$, and (c) $f = 0.55$. (d) is the early portion of (c) and compares two simulations with different distance between the shock and the outflow boundary (dots: shorter distance; see the text). Time is normalized to a half-reaction timescale of a steady-state detonation.
weakening of the primary detonation (times 7–12). Spontaneous reaction wave and the secondary detonation in post-shock matter behind the weakening leading shock (times 1–6); (b) re-establishment and subsequent

1. At this moment the new oscillation cycle begins.

Generation of a spontaneous wave and the subsequent transition to a detonation in compressed matter occurs via the Zeldovich gradient mechanism (Zeldovich et al. 1970; Lee & Moen 1980) in which the pressure wave is amplified by the energy release source which travels with the spontaneous velocity $D_{sp} = \left( \frac{\partial \tau(T(x))}{\partial x} \right)^{-1}$, where $\tau(T)$ is the energy release reaction timescale. For an efficient amplification of a pressure wave, $D_{sp}$ must be comparable to or exceed the local speed of sound, and the spontaneous reaction source must act for a sufficient period of time. The diminishing of the temperature gradient caused by the weakening of the leading shock favors both these requirements.

Since $\tau$ is an exponential function of $T$, the size of the reaction zone during the minimum of the detonation cycle depends exponentially on $f$. For $f = 0.71$, the increase of the reaction zone at the minimum of oscillations is much less pronounced than for $f = 0.62$. As a result, $D_{sp}$ becomes smaller and the generated pressure wave is weak and does not transition to a secondary detonation before it reaches the leading shock. In this case we observe a low amplitude, nearly sinusoidal oscillating behavior of a detonation wave. With decreasing $f$ the length of the reaction zone at minimum increases dramatically. In the D case $f = 0.55$ the reaction zone rapidly separates from the leading shock and the distance between the shock and the reacted matter becomes much larger than the length of the computational domain $L$. In this case, we observe the decay of the detonation wave but the re-ignition and formation

4.2. Oscillation Cycle

Figures 8–10 show the distributions of pressure, temperature, and carbon mass fraction inside the reaction zone at different moments of time during the third cycle of oscillations (Figure 7(b)) for the detonation $\rho_0 = 3 \times 10^6$ g cm$^{-3}$ and $f = 0.62$. During the minimum of post-shock pressure, times $t_5$ to $t_3$, the leading shock is weakened and the post-shock temperature is smaller than the corresponding steady-state post-shock temperature. As a result the reaction zone is approximately 10 times wider than $x_c$.

An important consequence of the widening of the reaction zone is the decrease of the gradients of temperature and reactivity of matter behind the leading shock. Flattening of the gradient of reactivity causes the development of a supersonic spontaneous reaction wave behind the leading shock between times $t_3$ and $t_4$. The emergence and amplification of the spontaneous wave are clearly visible in Figure 8 at $t_4$ and $t_5$ as a growing peak of pressure propagating to the right. Between $t_5$ and $t_6$ the forward part of the spontaneous wave steepens into a shock and the spontaneous wave transforms into a secondary detonation wave which propagates through the shocked and compressed un-reacted matter toward the leading shock.

Between $t_6$ and $t_7$ the secondary detonation overcomes and interacts with the leading shock and passes into the cold unburned matter where it becomes the main detonation wave. The interaction of the secondary detonation with the leading shock generates a rarefaction wave which travels back into the burned material. The rarefaction leads to a gradual weakening of the leading shock and widening of the reaction zone ($t_8$ to $t_{12}$). By the time $t_{12}$ the leading shock is weakened to such a degree that the distribution of physical parameters behind the shock resembles the distribution which existed in the beginning of the oscillation cycle at time $t_4$. At this moment the new oscillation cycle begins.

Figure 8. Oscillation cycle of the $f = 0.62$ C-detonation at $\rho_0 = 3 \times 10^6$ g cm$^{-3}$ shown in Figure 7(b). Plots of pressure, $P(x)$, for various moments of time during the third cycle. Distance is normalized to a half-reaction length-scale of a steady-state detonation. Times are (1) 113.2, (2) 124.3, (3) 134.1, (4) 136.2, (5) 137.5, (6) 137.9, (7) 138.8, (8) 139.2, (9) 139.6, (10) 142.2, (11) 174.5, (12) 183.1; normalized to a half-reaction timescale of a steady-state detonation. (a) Formation of the spontaneous reaction wave and the secondary detonation in post-shock matter behind the weakening leading shock (times 1–6); (b) re-establishment and subsequent weakening of the primary detonation (times 7–12).
of a spontaneous wave are significantly delayed and are not observed.

4.3. Re-ignition Time

We now proceed to estimate a characteristic timescale of re-ignition for D-type detonations. Figure 11 illustrates the D-type behavior of a detonation with \( \rho_0 = 3 \times 10^6 \) g cm\(^{-3}\) and \( f = 0.55 \). In this case the initial perturbations grow and then the reaction zone rapidly separates from the leading shock. The post-shock pressure decreases from the initial values \( P \simeq 13P_0 \) (time \( t_1 \)) to \( P \simeq 8P_0 \) at \( t_7 \) and temperature from \( T_s \simeq 2.6 \times 10^9 \) K to \( T_s \simeq 1.8 \times 10^9 \) K. By the time \( t_7 \) the detonation pressure spike
Figure 11. Propagation of a detonation wave for $\rho_0 = 3 \times 10^6$ g cm$^{-3}$ and $f = 0.55$. The figure shows the development of the instability and separation of the reaction zone from the leading shock. Distance is normalized to a half-reaction length-scale of a steady-state detonation. Times are (1) 115.6, (2) 134.1, (3) 136.2, (4) 137.5, (5) 137.9, (6) 138.4, (7) 138.8; normalized to a half-reaction timescale of a steady-state detonation.

disappears and the pressure in the shocked material becomes constant and approximately equal to the pressure $P_d$ of the corresponding steady-state detonation.

The re-ignition time can thus be estimated as follows. For a given $\rho_0$ and $f$ we first calculate the detonation pressure $P_d$ assuming $q_d = q_C$. Next, we calculate the post-shock temperature $T_s$ and post-shock density $\rho_s$ of a shock with the post-shock pressure $P_s = P_d$. Finally, using the values of $T_s$, $\rho_s$, and the initial carbon composition $Y_{C,0}$ we calculate the timescale $\tau_C(T_s, \rho_s, Y_{C,0})$ for the leading C$^{12}$ + C$^{12}$ reaction. This time serves as an estimate of the re-ignition time.

We calculate $\tau_C$ as follows. The kinetic of the C$^{12}$ + C$^{12}$ reaction may be approximated as

$$\frac{dY_C}{dt} = -R_C(\rho, T, Y_C) = -A\rho Y_C^2 e^{-Q/\tau_1^{1/3}}, \quad (13)$$

where $Q \simeq 84.165 \times 10^3$ K$^{1/3}$, $T_a = T/(1 + 0.067 \times 10^{-9}T)$, and $A(T)$ is a known weak (non-exponential) function of temperature (Fowler et al. 1975).

In what follows the subscript $i$ indicates initial physical values at the beginning of the reaction. The $e$-folding time of C$^{12}$ + C$^{12}$ reaction is

$$\tau_C^{-1} = -\frac{1}{Y_{C,i}} \frac{dY_{C,i}}{dt} = \left(\frac{R_C}{Y_{C,i}}\right) \quad (14)$$

if we assume that the reaction occurs at constant $T = T_i$ and $\rho = \rho_i$. To evaluate the actual timescale $\tau_C$ we must take into account self-acceleration of the C$^{12}$ + C$^{12}$ reaction caused by increase of $T$.

The evolution of $T$ is governed by

$$\frac{dT}{dt} = \left(\frac{\partial T}{\partial \epsilon}\right) \left(\frac{q_C}{Y_{C,i}}\right) R_C(T, \rho, Y_C), \quad (15)$$

where $q_C$ is the energy release in C$^{12}$ + C$^{12}$ reaction per unit mass of CO mixture with initial carbon composition $Y_{C,i}$. Using the Frank-Kamenetskii (1967) (FK) approximation we assume that all values in Equation (15) can be evaluated at constant initial conditions except the exponent in $R_C(T)$. In the FK approximation we can re-write Equation (15) as

$$\frac{dT}{dt} \simeq \left(\frac{T_i}{\tau_T,i}\right) \exp\left(\frac{Q}{T_i^{1/3}} - \frac{Q}{T_a^{1/3}}\right)$$

$$\simeq \left(\frac{T_i}{\tau_T,i}\right) \exp\left(\frac{1}{\Theta} \left(\frac{T}{T_i} - 1\right)\right), \quad (16)$$
Figure 12. Solid circles: estimated re-ignition length-scale; open circles: estimated re-ignition timescale (see Section 4.3). Horizontal dashed line: characteristic spatial scale of an exploding Chandrasekhar-mass CO white dwarf.

where

\[ \tau_{T,i} = \left( \frac{\epsilon_i}{q_C} \right) \left( \frac{d \ln \epsilon_i}{d \ln T_i} \right) \tau_{C,i} \]  \hspace{1cm} (17)

is the temperature \( e \)-folding time evaluated at constant initial conditions and

\[ \Theta = \left[ \frac{3}{\tau_{T,i}} \right] \left( \frac{T_i}{T_{ai}} \right) \]  \hspace{1cm} (18)

is the FK factor. Integration of Equation (16) gives

\[ \tau_C \simeq \tau_{T,i} \int_{T_i}^{\infty} \exp \left( -\Theta \left( \frac{T}{T_i} \right) - 1 \right) d \left( \frac{T}{T_i} \right) = \Theta \cdot \tau_{T,i}. \]  \hspace{1cm} (19)

Formally, the upper limit in the integral (19) should be equal to some final temperature \( T_f > T_i \) reached at the end of burning. \( T_f \) may be replaced with \( \infty \) since the integral in Equation (19) is mostly accumulated at temperatures \( T \simeq T_i \). FK factor \( \Theta \) in Equation (19) characterizes shortening of the reaction timescale due to self-acceleration of burning. We note that in the FK approximation

\[ \left( \frac{d \ln R_i}{d \ln T_i} \right) \simeq \frac{1}{\Theta} \]  \hspace{1cm} (20)

so that \( \tau_C \) may also be written as

\[ \tau_C(T_i) \simeq \left( \frac{\epsilon_i}{q_C} \right) \left( \frac{d \ln \epsilon_i}{d \ln T_i} \right) \left( \frac{d \ln T_i}{d \ln R_i} \right) \tau_{C,i}. \]  \hspace{1cm} (21)

Figure 12 shows temporal and spatial re-ignition scales as a function of \( \rho_0 \) which were estimated for the borderline D-cases (see Table 1 and dashed line in Figure 6). Both scales increase exponentially with decreasing \( \rho_0 \). At densities less than \( \simeq 10^9 \text{ g cm}^{-3} \) the timescale becomes greater than the explosion time of a white dwarf (\( \simeq 1 \text{ s} \)) and the spatial scale, estimated by multiplying the velocity of the leading shock of the detonation with the re-ignition time, becomes greater than the scale of the exploding white dwarf. At these densities the one-dimensional propagation of a C-detonation will be impossible.

4.4. Stability Criterion

In general, the instability is a consequence of a positive feedback between the hydrodynamical perturbations and the temperature-dependent energy release inside the detonation wave. The feedback loop consists of three parts. First, the temperature perturbation leads to the increase of the reaction rate. This effect depends on the sensitivity of \( R \) to \( T \). Second, the increase of \( R \) leads to the increase of the energy generation rate. This effect is proportional to the amount of nuclear energy which is released by burning. Third, the increase in the energy generation leads to a faster rise of \( T \). The latter effects depend on specific heat of matter. For illustration, consider a thermally isolated, uniform fluid element of a carbon–oxygen mixture at constant volume. The evolution of \( T \) in the element is described by Equation (15). To compare the feedback loop for fluid elements with different initial temperatures and densities we scale \( t \) to the timescale \( \tau_{C,i} \) which is required to burn half of initial carbon at constant initial conditions (see Equation (14)). Then in FK approximation Equation (15) becomes

\[ \frac{dT}{dt} = T_i \left( \frac{\partial \ln T_i}{\partial \ln \epsilon_i} \right) \left( \frac{q_C}{\epsilon_i} \right) \frac{R_C(T, \rho, Y_{C,i})}{R_C(T_i, \rho_i, Y_{C,i})}, \]  \hspace{1cm} (22)

where \( \tilde{t} = t / \tau_{C,i} \).

Consider now two identical fluid elements, one with initial temperature \( T_i \) and another one with perturbed initial temperature \( T_i + \Delta T, \Delta T \ll T_i \). The evolution of \( \Delta T \) with \( \tilde{t} \) is given by

\[ \frac{d\Delta T}{d\tilde{t}} = \frac{d(T + \Delta T)}{d\tilde{t}} - \frac{dT}{d\tilde{t}} \simeq \left( \frac{\partial \ln T_i}{\partial \ln \epsilon_i} \right) \left( \frac{q_C}{\epsilon_i} \right) \left( \frac{\partial \ln R_i}{\partial \ln T_i} \right) \Delta T. \]  \hspace{1cm} (23)

Hence \( \Delta T(\tilde{t}) \propto \exp(\beta \tilde{t}) \) where the increment

\[ \beta = \beta(T_i, \rho_i, Y_{C,i}) = \left( \frac{\partial \ln R_i}{\partial \ln T_i} \right) \left( \frac{q_C}{\epsilon_i} \right) \left( \frac{\partial \ln T_i}{\partial \ln \epsilon_i} \right). \]  \hspace{1cm} (24)

We see that the increment is the product of three dimensionless factors. The first factor in Equation (24) describes the sensitivity
of \( R \) to temperature, the second factor characterizes the relative energy content of the fuel, and the third takes into account specific heat of matter.

Table 1 gives \( \beta \) and individual multipliers in Equation (24) for computed detonations. Inspection of the table shows that variations of \( \beta \) with \( \rho_0 \) and \( f \) are mostly caused by variations of the second and third multipliers in Equation (24). For example, for \( \rho = 10^7 \text{ g cm}^{-3} \) the value of \( \beta \) varies by a factor of \( \approx 2.90 \) for \( f \) varying from 1 to 0.61, \( q_c/\epsilon_c \), and \( (\partial \ln T/\partial \ln \epsilon) \) vary by a factor \( \approx 1.6 \) whereas \( (\partial \ln R/\partial \ln T) = \Theta^{-1} \) varies by a factor of only \( \approx 1.1 \). The situation is similar for other densities, as well. The reason for the large variations of the second and the third multipliers is related to the dependence of internal energy per unit mass and specific heat of degenerate matter on \( \rho \). On the other hand, \( \Theta^{-1} \) is density independent (screening corrections at post-shock temperatures are small and can be neglected) and is a weak function of temperature, \( \Theta^{-1} \sim T^{-1/3} \). As a result, relative variations of \( \Theta^{-1} \) are small and this factor does not contribute to the variations of \( \beta \) significantly.

We note that the relative importance of the factors controlling the instability of a detonation is different in C-detonations in SNe and in terrestrial detonations in reactive gases. The equation of state for terrestrial gases (for example Burcat & Ruscic 2005) is such that \( \epsilon_c \) is usually independent of \( \rho \) and increases with \( T \) linearly or faster (e.g., Burcat & Ruscic 2005). Specific heat in reactive gases is also density independent and may be a constant of \( \rho \). As a result, the sensitivity of chemical reaction rates on \( T \) play a significant role for terrestrial detonations.

Close inspection of Table 1 shows that the transition from stable to unstable behavior of a C-detonation with decreasing \( f \) wave typically occurs for \( \beta \approx 9-10 \), virtually independent of \( \rho_0 \). The borderline between O-type and D-type detonations corresponds to \( \beta \approx 14-15 \). Of course, the correlation is not perfect. Perfect correlation should not be expected since the detonation wave is a distributed system in which physical conditions vary inside the reaction zone. Communication of information from one point to another involves interaction of many fluid elements and occurs with a finite speed. Derivation of Equation (24) is done within a simple one-zone model and does not take any of this into account. Nevertheless, it seems that the derivation catches a significant part of the feedback.

Finally, the feedback analysis helps to understand why detonation in degenerate carbon–oxygen tends to become more unstable at higher densities. The leading part of a complete CO detonation can be viewed as a C-detonation overdriven to \( f > 1 \). The feedback loop consideration applies to this detonation as well. With increasing \( \rho_0 \) specific heat of degenerate matter decreases drastically and as a result \( (\partial \ln T/\partial \ln \epsilon) \) in Equation (24) increases by a factor of almost \( \approx 10 \) (see Table 1). This leads to a noticeable increase of the strength of the feedback loop. As a result, greater overdrive is needed for stabilizing the detonation and the stability boundary passes through the overdriven detonation regimes (Section 4.1 and Figure 6).

5. DISCUSSION AND CONCLUSIONS

In this paper, we studied the basic properties and one-dimensional stability of incomplete carbon–oxygen detonations in low-density environments of SNe Ia. Calculations of the steady-state structure of C-detonations show that a Chapman–Jouguet C-detonation has a velocity \( D_{CJ} \) which is a factor of \( \approx 20\%−25\% \) smaller than the CJ velocity of a complete NSE detonation \( D_{CJ, NSE} \). This decrease translates into a decrease of the post-shock temperature by a factor \( \approx 0.7 \) (Table 1), and a corresponding increase of the half-reaction thickness \( x_c \) by a factor \( \approx 30−100 \) (Figure 5). The half-reaction timescale \( t_c \simeq x_c/D \) increases by approximately the same factor. While the increase is appreciable, at all relevant densities \( x_c \) still remains relatively small compared to the characteristic scale of a WD \( \approx 10^{8} \) cm.

Decreased energy release in C-detonations has a major effect on the detonation stability. In contrast to complete detonations which are one-dimensionally stable at low densities, C-detonations are highly one-dimensionally unstable. The boundary of stability for C-detonations (Figure 6) passes through detonation regimes which are overdriven with respect to CJ C-detonation. Near the boundary of stability, unstable detonations exhibit low-amplitude pulsations and have a continuous distribution of physical parameters inside the reaction zone. With decreasing overdrive the detonation becomes highly unstable and begins to propagate by periodically generating a spontaneous reaction wave inside the primary reaction zone. The spontaneous wave transitions to a secondary detonation which overcomes and accelerates the leading detonation shock. The subsequent decay and the separation of the leading shock from the reaction zone gives rise to a new spontaneous wave and starts the next oscillation cycle.

Transition from stable to unstable behavior, the level of instability, and the length of the detonation cycle depend mainly on specific heat and internal energy of degenerate matter behind the leading shock. The sensitivity of reaction rates to post-shock temperature is less important. This is in contrast with idealized Arrhenius detonations whose stability is usually highly dependent on the sensitivity of the reaction rate to temperature (e.g., Lee & Stewart 1990). The stability and detonation cycle of a C-detonation in an SN Ia cannot be understood without taking effects of the equation of state of degenerate matter into account.

The thickness of a steady-state one-dimensional detonation wave (Figure 5) can be used to estimate the minimal resolution required for a correct description of the detonation structure and detonation stability. The absolute minimum of numerical resolution can be no less than \( n \approx 10−30 \) computational cells per \( x_c \). The minimal spatial resolution \( \Delta \rho \) depends on background conditions in unburned matter and can be estimated for a given density and overdrive by taking \( x_c \) from Figure 5 and dividing it by \( n \). Even for the most favorable case of a CJ C-detonation at \( \rho_0 = 10^6 \text{ g cm}^{-3} \) (the upper left end of the solid line for \( \log \rho_0 = 6 \) in Figure 5) and \( n = 10 \) the required resolution \( \delta \rho \approx 10^5 \text{ cm} \) is significantly less than the resolution of current global three-dimensional simulations of SNe Ia. For one-dimensional lagrangian simulations we can estimate the relative mass resolution \( \delta \rho = \delta M/M_{WD} \) as

\[
\delta \rho \simeq \frac{4\pi \rho_0 R^2 x_c}{n M_{WD}} \simeq 10^{-5} \left( \frac{R}{5 \times 10^8 \text{ cm}} \right)^2 \left( \frac{x_c}{10^3 \text{ cm}} \right) \left( \frac{M_{\odot}}{M_{WD}} \right) \left( \frac{10}{n} \right) \left( \frac{\rho_0}{10^6 \text{ g cm}^{-3}} \right),
\]

where \( M \) is the Lagrangian mass coordinate and \( R \) is the radius of a spherical layer with density \( \rho_0 \) at the moment of time when the detonation is passing through the layer. For \( \rho_0 = 10^6 \text{ g cm}^{-3} \), \( R \approx 5 \times 10^8 \text{ cm} \) (see below), and \( n = 10 \) we obtain \( \delta \rho \simeq 10^{-5} \).

The period and spatial scale of the detonation cycle of a C-detonation increase with decreasing density. For \( \rho \leq \rho_0 \) the resulting half-reaction thickness \( x_c \) and velocity \( D \) increase (Figures 5 and 6), leading to an increased sensitivity of the reaction rates to post-shock temperatures. The instability of C-detonations increase with decreasing density as well (Figure 5) with the sensitivity increasing by a factor of \( \approx 10 \) (see Table 1). The increase is appreciable, at all relevant densities \( x_c \) still remains relatively small compared to the characteristic scale of a WD \( \approx 10^{8} \) cm.
$10^6$ g cm$^{-3}$ the period becomes larger than the explosion timescale, $\sim 1$ s, of a white dwarf, which suggests that the influence of the instability on propagation and quenching of a C-detonation wave could be significant at these densities. This may alter the composition of the outer layers. In particular, quenching at higher densities may leave more unburned carbon. From the observational point of view it would be important to estimate the velocity range of an SN Ia envelope which may be affected. This depends, of course, on a particular explosion model. For illustration, we give estimates for two DD models of Höflich et al. (2002). For a normal SN we take the DD model SP0022.20 with total mass $M_{WD} = 1.346 M_{\odot}$ and Ni$^{56}$ mass $M_{Ni} = 0.54 M_{\odot}$. In this model the detonation wave, which propagated outward through the WD already pre-expanded by deflagration, passed through the layer with density $\rho_0 = 10^6$ g cm$^{-3}$ when the layer was located at the mass coordinate $M = 1.300 M_{\odot}$ and radius $R \approx 5 \times 10^8$ cm. At this moment of time the layers with density $\rho < 5 \times 10^8$ g cm$^{-3}$ had radii $R \geq 5.6 \times 10^8$ cm. From this we estimate the characteristic scale of density variation at these densities as $L \approx (5 \times 10^8$ cm$)^{-1} \approx 5 \times 10^7$ cm. The corresponding timescale of density variation can be estimated by dividing $L$ by the difference in the expansion velocities of the layers $\approx 10^6$ cm s$^{-1}$ which gives the characteristic timescale $\approx 0.5$ s. The numbers are consistent with the values of $10^8$ cm and 1 s used in our general analysis in Sections 3 and 4, and in this section above. After the explosion and acceleration to free expansion, the layer with $\rho_0 = 10^6$ g cm$^{-3}$ was accelerated to $V \approx 23,000$ km at infinity. From this we conclude that the one-dimensional instability in a normal DD explosion may affect the outer 0.04 $M_{\odot}$ or 3% of an SN Ia envelope with velocities $V \geq 23,000$ km s$^{-1}$ at infinity. For a sub-luminous DD model SP0222.8 similar analysis shows that the instability may affect outer 0.08 $M_{\odot}$ or 6% of the envelope with velocities $V \geq 14,000$ km s$^{-1}$. Thus, the instability may affect the spectra and the light curve of these SNe before and near maximum light. We note that the mass resolution of the models was $\delta q \approx 10^{-3}$, i.e., two orders of magnitude greater that the resolution required for detecting the detonation instability.

In conclusion, we stress that this study is one dimensional and we caution that the above estimates are preliminary. In addition to a strong one-dimensional instability the detonation will be affected by transversal instability (e.g., Gamezo et al. 1999), curvature of the detonation front (e.g., Sharpe 2001), and spatial variations of the background density. Transverse instability is caused by the same feedback between the energy generation and temperature fluctuations which is responsible for the one-dimensional longitudinal instability. Other effects depend on the strength of the feedback, as well. Thus, incomplete C-detonations should be expected to be more unstable and more sensitive to the above-mentioned effects than the complete detonations. Investigation of the multi-dimensional behavior of C-detonations will be reported in the next paper (A. Khokhlov & I. Domínguez 2011, in preparation).

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APPENDIX

NUMERICAL METHOD

A.1. Numerical Approach

The Equations (1)–(4) are integrated using an adaptive mesh refinement (AMR) reactive flow fluid dynamic code ALLA (Khokhlov 1998). Reaction terms are coupled to fluid dynamics by time step splitting. During the hydrodynamical sub-step the Euler equations are integrated with $R = \dot{q} = 0$ using an explicit, directional-split, second-order accurate, Godunov-type conservative scheme with a Riemann solver (Colella & Glaz 1985), and a monotone VanLeer reconstruction (van Leer 1979).

Hydrodynamical time step is selected using the Courant number $= 0.9$. During the reaction sub-step the kinetic equations together with the equation of energy conservation, differential equations

$$ \frac{d\tilde{Y}}{dt} = \dot{R}, \quad \frac{d\tilde{\rho}}{dt} = \dot{\tilde{\rho}}, $$

(A1)

are integrated in each cell using a stiff solver with adjustable sub-cycling to keep the accuracy of integration of energy and composition to better than $10^{-3}$.

AMR is carried out at the level of individual cells. Size of computational cells at refinement level $l_{min} < l < l_{max}$ is $\Delta(l) = L \cdot 2^l$; where $l_{min}$ and $l_{max}$ are maximum and minimum levels of refinement, respectively. During the simulation the mesh is refined around the shocks, contact discontinuities, and in regions of large gradients of density, pressure, and mole fractions of $H^4$, $C^{12}$, $O^{16}$, $Ne^{20}$, $Mg^{24}$, and $Si^{28}$. Detected shocks and discontinuities are always refined to maximum level of resolution. Refinement based on chemical composition is used for species with concentrations $Y_i > 10^{-3}$. Further details of the refinement procedure can be found in Khokhlov (1998).

Calculations are performed in a reference frame moving with a constant velocity of a steady-state detonation $D$ in order to keep the detonation on the mesh as long as possible. A steady-state solution corresponding to a detonation velocity $D$ is mapped onto a computational domain of size $L$. A constant supersonic inflow with $u = -D$, $\rho = \rho_0$, $P = P_0$, and $Y = Y_0$ is imposed on the right boundary $x = L$. Zero-gradient boundary conditions are imposed at the left boundary $x = 0$. Calculations were performed with numerical resolution of $\approx 30$ cells per half-reaction length, $\Delta \approx x_C/30$, and $L \approx 100x_C$ and then repeated with two times lower numerical resolution and, when necessary, with up to four times higher numerical resolution and $L \approx (300–1000)x_C$ in order to confirm the observed detonation behavior.

A.2. Test Simulations

Linear stability and one-dimensional propagation of idealized detonations with the one-step Arrhenius kinetics and $\gamma$-constant equation of state,

$$ \frac{dY}{dt} = -Ye^{-\frac{Q}{T}}, \quad \frac{d\rho}{dt} = -d\frac{dY}{dt}, \quad P = (\gamma - 1)\rho \epsilon, \quad T = \frac{P}{\rho} $$

(A2)

where $Q$ is the activation energy, $q$ is the total energy release, and $\gamma = 1.2$, have been extensively studied in the past (Erpenbeck...
with the linear predictions. For $Q = 27$, interpolation in Table II of He & Lee (1995) gives $\sigma_f \simeq 0.470$. The simulations in Figure 13(d) give similar $\sigma_f \simeq 0.47$ in good agreement with the linear analysis and non-linear calculations of He & Lee (1995) (their Figure 10(b)). The instability of a detonation tends to increase with decreasing $f$. In agreement with He & Lee (1995), Williams et al. (1996), and Sharpe & Falle (2000) we found that the propagation of the above detonations becomes highly irregular when $f$ approaches $f = 1$.

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