The structure of detonation waves in supernovae revisited

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Abstract

The structure of a thermonuclear detonation wave can be solved accurately and, thus, may serve as a test bed for studying different approximations that are included in multidimensional hydrodynamical simulations of supernovae. We present the structure of thermonuclear detonations for the equal mass fraction of \(^{12}\text{C}\) and \(^{16}\text{O}\) (CO) and for pure \(^4\text{He}\) (He) over a wide range of upstream plasma conditions. The lists of isotopes we constructed allow us to determine the detonation speeds, as well as the final states for these detonations, with an uncertainty of the percent level (obtained here for the first time). We provide our results with a numerical accuracy of \(\sim 0.1\%\), which provides an efficient benchmark for future studies. We further show that CO detonations are pathological for all upstream density values, which differs from previous studies, which concluded that for low upstream densities CO detonations are of the Chapman–Jouget (CJ) type. We provide an approximate condition, independent of reaction rates, that allows to estimate whether arbitrary upstream values will support a detonation wave of the CJ type. Using this argument, we are able to show that CO detonations are pathological and to verify that He detonations are of the CJ type, as was previously claimed for He. Our analysis of the reactions that control the approach to nuclear statistical equilibrium, which determines the length-scale of this stage, reveals that at high densities, the reactions \(^{11}\text{B} + p \rightarrow ^{3}\text{He}\) play a significant role, which was previously unknown.

Key words: hydrodynamics – shock waves – supernovae: general

1 Introduction

Thermonuclear detonation waves are believed to play a key role in supernovae (Hoyle & Fowler 1960; Fowler & Hoyle 1964). The detonation wave structure is important for the energy release and for the nucleosynthesis during the explosion, and it is therefore a crucial ingredient for supernovae modelling (see Seitenzahl & Townsley 2017, for a recent review). However, resolving the detonation wave structure in a multidimensional hydrodynamical simulation of a supernova is currently impossible. This is because the fast thermonuclear burning dictates a burning length-scale that is much smaller than the size of the star, and because the number of isotopes participating in the thermonuclear burning is very large. These problems led to the introduction of various approximations that allow multidimensional hydrodynamical simulations of full stars. The error introduced by these approximations, however, is not well understood. Most notably, a small number (10 – 20) of isotopes is usually included in the multidimensional hydrodynamical simulations, and the method for choosing these isotopes has not yet been firmly established.

A relevant, much simpler, problem to analyse is the structure of a steady-state, planar detonation wave, given by the ZND theory (Zel’Dovich 1940; von Neumann 1947; Döring 1943), on which we concentrate in this work. This problem can be solved accurately for the case of a thermonuclear detonation wave, and thus can serve as a test bed for studying different approximations that are included in multidimensional hydrodynamical simulations. For example, we can calibrate lists of isotopes that allow the calculation of a thermonuclear detonation wave with some prescribed accuracy. We assume that the reader is familiar with the basic physics of thermonuclear detonation waves, as this topic has been heavily discussed over the past several decades. The theory of detonation waves in general is described in the text book of Fickett & Davis (1979) and the fundamental physics of thermonuclear detonation waves is discussed by Khokhlov (1989).

We consider two compositions for the upstream plasma that show dramatic differences in the structure of the detonation wave and are both relevant for supernova modelling. The first one is the equal mass fraction of \(^{12}\text{C}\) and \(^{16}\text{O}\) (CO) and the second is pure \(^4\text{He}\) (He). Other variants of the initial composition can be handled with the same tools described in this work.

The structure of steady-state, planar, thermonuclear detonation waves has been studied by numerous authors. Imshennik & Khokhlov (1984) studied detonation waves in pure \(^{12}\text{C}\), Khokhlov (1989) studied detonation waves in CO and He, and Townsley et al. (2016) presented solutions for detonation waves in CO (with a small initial mass fraction of \(^{22}\text{Ne}\)). Other studies employed a simplified reaction network (usually an...
α-net composed of 13 isotopes) to calculate steady-state, planar detonation waves in different mixtures (Bruenn & Marroquin 1975; Sharpe 1999; Gamezo et al. 1999; Dursi & Timmes 2006; Noel et al. 2007; Dominguez & Khokhlov 2011; Townsley et al. 2012; Dunkley et al. 2013). Since the final state of thermonuclear detonation waves can be dominated by isotopes that are not α-elements, the uncertainty with using α-net can be significant. Sharpe (1999) studied detonation waves in CO with a specific emphasis on a method to traverse the pathological point.

One of our objective here is to calculate Chapman–Jouget (CJ) detonations with an uncertainty in the order of the percent level over a wide range of upstream plasma conditions that are relevant for supernovae. The parameters of CJ detonations have been already calculated for CO (Bruenn 1971; Khokhlov 1988) and He (Mazurek 1973b; Khokhlov 1988). By comparing our results to those of previous works, we demonstrate that we are the first to reach an uncertainty level of 1 percent. In fact, we show that the equation of state (EOS) used by Mazurek (1973b) is not accurate enough, and that the EOS used by Khokhlov (1988) is apparently inconsistent with other available EOSs. Timmes & Niemeyer (2000) calculated a few properties for CJ detonations in He, and they claim to agree with the results obtained by Mazurek (1973b) and Khokhlov (1988). Although Timmes & Niemeyer (2000) do not provide the required information to reproduce their results, they probably did not use a tight criteria for agreement, as advocated here, to expose the apparent inconsistencies of Mazurek (1973b) and Khokhlov (1988).

We further calculate the structure of the detonation waves for both CO and He. Our determination of the pathological detonation speed for CO, as well as the final state of these detonations, is with a level of uncertainty of the percent level. We show that previous studies of the detonation wave structure with a detailed reaction network for both CO (Khokhlov 1989; Townsley et al. 2016) and He (Khokhlov 1989) are less accurate. Our results for the detonation wave speeds and for the final states are reported with a numerical accuracy of ~0.1%, representing an efficient benchmark for future studies. We provide all the relevant information needed to fully reproduce our results.

Besides providing accurate results and highlighting a few shortcomings of previous works, we present here a few new insights into the structure of thermonuclear detonation waves. We show that CO detonations are pathological for all upstream densities values, as far as our numerical accuracy allows us to test this. This is different from previous studies (Imshennik & Khokhlov 1984; Khokhlov 1989; Sharpe 1999; Gamezo et al. 1999; Dunkley et al. 2013), which concluded that for low upstream densities, CO detonations are of the CJ type. We explain why these claims were probably due to a loose definition for burning completion and/or low numerical accuracy. We provide an approximate condition, independent of reaction rates, that allows to estimate whether arbitrary upstream values (including composition) will support a detonation of the CJ type. Using this argument, we are able to show that CO detonations are pathological for all upstream densities and to verify that He detonations are of the CJ type, as was previously claimed for He (Khokhlov 1989). We show conclusively for the first time that in the case of CO detonations, the sonic point changes position in a discontinuous manner from \( x \sim 100 \text{cm} \) to \( x \sim 10^6 \text{cm} \) around the upstream density of \( \approx 2.7 \times 10^7 \text{g cm}^{-3} \).

The calculations in this work were performed with a modified version of the MESA code\(^1\) ( Paxton et al. 2011, 2013, 2015).

The definition of the problem to be solved is described in Section 2. The required input physics for an accurate calculation of the detonation wave structure is described in Section 3. We study CJ detonations in Section 4 and the full structure of the detonation waves in Section 5. We discuss the approximate condition needed in order to estimate whether arbitrary upstream values will support a detonation of the CJ type in Section 6 and the role of weak reactions in Section 7. We summarize our results in Section 8.

2 DEFINITION OF THE PROBLEM

The structure of a detonation wave can be found by integration, where the initial conditions are the downstream values of the leading shock. We assume that the pressure, \( P \), and the internal energy per unit mass, \( ε \), are given as a function of the independent variables: density, \( ρ \), temperature, \( T \), and the mass fraction of the isotopes, \( X_i \) (\( i = 1 \) and, unless stated otherwise, the sum goes over all isotopes). For planar, steady-state, non-relativistic hydrodynamics, the equations to integrate are (see e.g. Khokhlov 1989):

\[
dP = \left( \frac{\partial P}{\partial T} \right)^{-1} \left[ dq - \sum_i \left( \frac{\partial P}{\partial X_i} \right) dX_i \right] + \sum_i \left( \frac{\partial P}{\partial X_i} \right) dX_i,
\]

\[
dT = \left( \frac{\partial P}{\partial T} \right)^{-1} \left[ \frac{\partial P}{\partial \rho} d\rho - \sum_i \left( \frac{\partial P}{\partial X_i} \right) dX_i \right],
\]

where \( c_s \) is the frozen (constant composition), non-relativistic speed of sound, \( u \) is the velocity in the shock rest frame

\[
u = \frac{\rho_0}{\rho} D,
\]

\( \rho_0 \) is the upstream density, \( D \) is the shock velocity in the lab frame (in which the upstream fuel is at rest), \( q \) is the average binding energy:

\[
q = N_A \sum_i Q_i Y_i,
\]

\( Q_i \) are the binding energies of the nuclei, \( Y_i \equiv X_i / A_i \), the molar fractions of the nuclei (see discussion in Section 2.1), \( A_i \) are the nucleon numbers and \( N_A \) is Avogadro’s number. Upstream values will be denoted with subscript 0, CJ values with subscript CJ and pathological values with subscript *. We further define the equilibrium speed of sound, \( c_s^* \). Unless stated otherwise, the partial derivatives are taken with the rest of the independent variables remaining constant. Sharpe (1999) pointed out that since \( \sum_i X_i = 1 \), not all \( X_i \) are independent, and he consequently eliminated from the integration the mass fraction of one isotope and instead determined it from \( \sum_i X_i = 1 \). In this paper, we choose to treat all \( X_i \) as independent variables, while using \( \sum_i X_i = 1 \) only for the initial conditions. This approach is valid, since the equations that determine \( dX_i \) must satisfy \( \sum_i dX_i = 0 \), leading to \( \sum_i X_i = 1 \) throughout the integration, up to a numerical error that can be controlled. Equations (1)-(3) are accurate as long as there is no heat transfer nor particle exchange with the environment. Specifically, these equations assume the absence of weak reactions.

The form of Equations (1) demonstrates that following some change in composition \( dX_i \) that determines some nuclear energy

\(^1\) version r7624; https://sourceforge.net/projects/mesa/files/releases/
release $dq$) the changes in $dp$ and $dT$ are independent of the rate in which this change took place. It follows that if all reaction rates are slower by some factor, then the fluid reaches the exact same state but over a time longer by the same factor. The burning limiter for hydrodynamical simulation suggested by Kushnir et al. (2013) multiplies all reaction rates by some factor to prevent unstable numerical burning and, therefore, accurately describes detonation waves over scales larger than those in which the limiter operates.

In order to calculate the structure of the detonation wave, a full derivative in time of Equations (1) is taken:

$$\frac{dp}{dt} = \frac{\partial P}{\partial T} \left( \frac{\partial u}{\partial T} - \sum_i \frac{\partial P}{\partial X_i} \frac{dx_i}{dt} \right) + \sum_i \frac{\partial P}{\partial X_i} \frac{dx_i}{dt}.$$  \hspace{1cm} (4)

The integration of Equations (4) yields the state of a fluid element as a function of the time since it was shocked, given the reaction rates

$$dx_i/dt = f_i(\rho, u, T, \{X_i\}).$$  \hspace{1cm} (5)

Equation (5) includes the complexity of the problem, as many isotopes have to be included in the integration with many reactions. We present our results as a function of the distance behind the shock wave, $x$, connected to the time through $u = dx/dt$.

We briefly mention here the possible solutions of Equations (4) (Wood & Salsburg 1960). In the final state of the detonation wave all isotopes are in equilibrium, i.e. $dx_i/dt = 0$ (for the case of a thermonuclear detonation wave, this state is nuclear statistical equilibrium (NSE), see Section 3.1). The equilibrium composition is a function of the thermodynamic variables only, so there exist an equilibrium Hugoniot adiabat that connects to the upstream values. For a given shock velocity, $D$, the Rayleigh line that passes through the upstream values either does not intersect the equilibrium Hugoniot, is tangent to it (one point of intersection), or intersects it twice. The shock velocity for which there is one intersection is called the CJ velocity, and it is independent of reaction rates. In this work we find $D_{\text{CJ}}$ as well as the corresponding equilibrium state, by numerically iterating over the value of $D$. If during the integration of Equations (4) with $D = D_{\text{CJ}}$ the flow is always subsonic, then the minimal possible shock velocity is $D_{\text{CJ}}$. However, if during the integration the flow becomes sonic, then from Equations (4), we must require $\phi = 0$ at the sonic point. The minimal shock velocity for which this condition is satisfied is called the pathological shock velocity, $D_{\text{P}}$, and it can only be found by integrating Equations (4) (and so it depends on reaction rates). Overdriven detonations, which are solutions with higher shock velocities than the minimal shock velocity, either $D_{\text{CJ}}$ or $D_{\text{P}}$, exist as well, and they are subsonic throughout the integration. It can be shown that for pathological detonations $\phi$ changes sign while crossing the sonic point. While $\phi$ can change sign multiple times along the integration, for all known examples of thermonuclear detonation waves, for CJ detonations $\phi > 0$ throughout the integration and for pathological detonations $\phi < 0$ following the sonic point crossing. We provide in Section 5.1.3 an example of a pathological detonation in which $\phi$ changes sign twice before the sonic point crossing. Finally, note that the equilibrium state is only approached asymptotically at an infinite distance behind the shock wave. As we discuss in Section 5, previous authors provide a finite distance behind the shock wave in which the equilibrium state is obtained, which could be due to a loose definition for burning completion.

We use the following definitions for the average nucleon number and proton number:

$$\bar{A} = \frac{1}{\sum_i X_i/A_i}, \quad \bar{Z} = \bar{A} \sum_i X_i/A_i,$$  \hspace{1cm} (6)

where $Z_i$ is the proton number of isotope $i$. We also define for the heavy isotopes:

$$\bar{Y} = \sum_{i, i \neq n, p, a} Y_i, \quad \bar{A} = \frac{1}{\sum_{i, i \neq n, p, a} X_i},$$  \hspace{1cm} (7)

It is convenient to normalize densities, $\rho_i = \rho(\text{g cm}^{-3})/10^7$, and temperatures, $T_0 = T[K]/10^9$.

2.1 The level of accuracy

We differentiate between the numerical accuracy (or convergence) of the results, which depends on the numerical scheme, and their uncertainty, which depends on the level of approximations that we introduce, as well as on the uncertainty of the input physics. Our aim, for a given set of input physics, is to reach a numerical accuracy of $\sim 10^{-3}$. This degree of numerical accuracy is appropriate for benchmarking and code checking. This numerical accuracy can be (and for many cases is) much higher than the uncertainty of the EOS and of the reaction rates that dominate the uncertainty budget.

The approximation of non-relativistic hydrodynamics is expected to introduce an error of MeV/$m_p c^2 \sim 10^{-3}$ for thermonuclear detonation waves. We further approximate the nuclear masses as $m_i \approx A_i m_{\text{u}}$, where $m_{\text{u}}$ is the atomic mass unit, unless stated otherwise. This approximation is always better than 1% for each isotope, and the relevant isotopes with significant errors are: $n$ (error of $\approx 8.6 \times 10^{-3}$), $p$ ($\approx 7.8 \times 10^{-3}$), $^2\text{H}$ ($\approx 7.0 \times 10^{-3}$), $^3\text{H}$ ($\approx 5.3 \times 10^{-3}$), $^3\text{He}$ ($\approx 5.3 \times 10^{-3}$), $^6\text{Li}$ ($\approx 2.5 \times 10^{-3}$), $^7\text{Li}$ ($\approx 2.3 \times 10^{-3}$) and $^7\text{Be}$ ($\approx 2.4 \times 10^{-3}$). Since the total mass fraction of these isotopes is at most a few percent under the conditions relevant for thermonuclear detonation waves, the approximation of $m_i \approx A_i m_{\text{u}}$ introduces an error smaller than $\sim 10^{-3}$. The total mass fraction of other isotopes with a similar significant deviation from $m_i \approx A_i m_{\text{u}}$ is always small. The level of error introduced by the absence of weak reactions is discussed in Section 7.

3 INPUT PHYSICS

3.1 Nuclear statistical equilibrium (NSE)

NSE is the unique nuclear composition of a system when strong and electromagnetic interactions are in a state of detailed balance for a given set of thermodynamic state variables and electron fraction. Applying a detailed balance to the reaction that breaks up a nucleus with a nucleon number $A_i$ and a proton number $Z_i$ into free nucleons ($A_i, Z_i) \leftrightarrow Z_i p + N_i n$, where $N_i \approx A_i - Z_i$, yields a relation between the chemical potential of the nucleus $\mu_i$ and the chemical potential of free protons $\mu_p$ and neutrons $\mu_n$: $\mu_i = Z_i \mu_p + N_i \mu_n$ (Clifford & Taylor 1965). The last relation can be written as

$$Z_i \mu_p + N_i \mu_n = m_i c^2 + k_B T \ln \left( \frac{n_i}{w_i(T)} \right) \frac{h^2}{2\pi m_i k_B T} \left( \frac{k_B T}{h^2} \right)^{3/2} + \mu_i^{\text{cond}},$$ \hspace{1cm} (8)

where $k_B$ is Boltzmann’s constant, $h$ is Planck’s constant, $n_i$ is the number density and $\mu_i^{\text{cond}}$ is a Coulomb interaction term.
(Calder et al. 2007; Seitenzahl et al. 2009). The Coulomb term and the conditions under which Equation (8) is valid are discussed in Section 3.4. The mass fractions of all nuclei in an NSE can therefore be expressed in terms of the chemical potential of the protons and the neutrons and the nuclear binding energies \( Q_i = (Z_i m_p + N_i m_n - m_i) c^2 \):\[ X_i = \frac{m_i}{\rho} w_i(T) \left( \frac{2 \pi m_i kT}{h^2} \right)^{3/2} \times \exp \left[ \frac{Z_i (\mu_p + \mu_n) c^2 + N_i \mu_n - \mu_i c^2 + Q_i}{kT} \right], \] (9) where \( w_i(T) \) are the nuclear partition functions and here we take the accurate nuclear masses for \( m_i \). Since the mass fractions of all nuclei sum to one, \( \sum_i X_i = 1 \), and the nuclear composition has the prescribed electron fraction, \( Y_e = \sum_i X_i Z_i / A_i \), for a given \( \rho \), \( T \), and \( Y_e \), the mass fractions of all the isotopes can be found by solving for the neutron and proton chemical potentials that satisfy the two constraints. The NSE state is found by using a modified version of the NSE routine of Frank Timmes\(^2\). Specifically, we include in Eq. (9) the ion–ion Coulomb interaction terms of Chabrier & Potekhin (1998, see detailed discussion in Section 3.4).

The nuclear masses and partition functions were taken from the file \textsc{winvnn\_v2.0\_dat}, which is available through the JINA reaclib data base\(^3\) (JINA, Cyburt et al. 2010). For those isotopes whose \( m_i \) values in \textsc{winvnn\_v2.0\_dat} differed from the most updated values given in the ENSDF database\(^4\), \( m_i \), we used the latter values instead\(^5\). The list of isotopes for which \( m_i \) and \( m_i \) differ is given in Table A1 of Appendix A, together with their mass (excess) values. The file \textsc{winvnn\_v2.0\_dat} provides the values of \( w_i(T) \) over some specified temperature grid in the \([10^8, 10^{10}] \) K range. For numerical stability, it is better to fit the \( w_i(T) \) values to some function rather than interpolate. We use the functional form suggested by Woosley et al. (1978):\[ w_i(T) = (2 J_{i,0} + 1) \left( 1 + \sum_k E_{i,k} \exp(-E_{i,k}/T_{9}) \right) \times \exp \left[ a_i/T_{9} + b_i + c_i T_{9} + d_i T_{9}^2 \right], \] (10) where \( (2 J_{i,0} + 1) \) is the statistical weight for the ground state of isotope \( i \) and \( a_i \) is negative. We initially used an extended list of 581 isotopes (see Table 1) to fit suitable sets of isotopes for the integration of Eqs. (4) (see Section 3.2). We could usually fit the nuclear partition function for the extended list of isotopes with \( E_{i,k} \) being equal to zero to better than 10\% over the relevant temperature range \([1.5 \times 10^8, 10^{10}] \) K. In the case that such a fit was not possible, low-lying excited levels with \( E_{i,k} \) and the excitation energy \( E_{i,k} \) [MeV] were added, where \( E_{i,k} = (2 J_{i,k} + 1)/(2 J_{i,0} + 1) \) and \( F_{i,k} = 11.6045 E_{i,k} \). The addition of, at most, three low-lying excited levels typically sufficed to fit to better than 10\%. For two isotopes, the fit was slightly worse: \( ^{72}\text{As} (-12.7\%) \) and \( ^{89}\text{Kr} (-19.6\%) \). The inaccuracies of the fit functions negligibly effect the results (see discussion in Section 4). We make the fit parameters for all isotopes publicly available\(^6\). We note that for some isotopes, the values of \( J_{i,0} \) in \textsc{winvnn\_v2.0\_dat} differ from the most updated values given in the ENSDF data base\(^7\). In these cases, we used the values of ENSDF, \( J_{i,0} \), and normalized the \( w_i(T) \) values from \textsc{winvnn\_v2.0\_dat} to \( w_i(T) \) as follows\(^8\):\[ w_i(T) = 1 + \frac{2 J_{i,0} + 1}{2 J_{i,0} + 1} (w_i(T) - 1). \] (11) The list of isotopes for which \( J_{i,0} \) and \( J_{i,0} \) differ is given in Table A2 of Appendix A, together with their spin values.

When nearing a state of NSE, the plasma may be in an intermediate state of nuclear-statistical-quasi-equilibrium (NSQE; Bodansky et al. 1968), in which a group of heavy isotopes are in detailed balance. We assume that at NSQE there is an equilibrium of neutrons, protons, and \( \alpha \)-particles, \( \mu_\alpha = 2 \mu_p + 2 \mu_n \), and that the rest of the isotopes are in a detailed balance, such that the chemical potentials of every two of them, \( i \) and \( j \), satisfy \( \mu_i - \mu_j = (N_i - N_j) \mu_n + (Z_i - Z_j) \mu_p \). In particular, under this assumption the state of NSQE is uniquely determined by specifying \( \rho, T, Y_e \), and \( Y \) (for a detailed discussion, see Khokhlov 1989).

3.2 Nuclear reaction network

Previous studies of thermonuclear detonation waves employed lists of isotopes that were considered extensive enough. However, this assumption was not backed up by any quantitative calculation, so one cannot estimate the error introduced by these lists of isotopes. Moreover, inclusion of irrelevant isotopes can decrease the numerical accuracy. We, therefore, aim at finding a reasonably short list of isotopes that allows the calculation of a thermonuclear detonation wave with some prescribed degree of accuracy. We first define an extended list of 581 isotopes (see Table 1), which includes all the available isotopes with \( Z \leq 14 \) from the file \textsc{winvnn\_v2.0\_dat} that satisfy the following two conditions:

(i) JINA includes strong reactions that connect the isotope to the bulk of the isotopes (say to \( ^{56}\text{Ni} \)). In other words, a subnet of a few isotopes is not allowed.

(ii) The isotope’s decay time is longer than 1 ns (which is roughly the carbon-burning time-scale in CO detonations).

We further add to our list of isotopes an extended pool of isotopes with \( Z > 14 \) that is sufficient in terms of the conditions described below. Next, given some minimal abundance \( Y_{\text{min}} \), we include in the list every isotope that has an NSE number abundance that is \( Y_i > Y_{\text{min}} \) for some \( \rho, T \) and \( Y_e \) within the ranges \( T \in [2 \times 10^8, 3 \times 10^{10}] \) K, \( \rho \in [100, 10 \times 10^{10}] \) g/cm\(^3\) and \( Y_e \in [0.495, 0.5] \). We obtained lists for a few values of \( Y_{\text{min}} = 10^{-3} \) (\( y = 4, 5, 6, 7 \)). These lists have to be supplemented with other isotopes that, while not represented in the NSE state, are significant for the burning process. Specifically, the relaxation to an NSE state is controlled by slow reactions between low-\( Z \) isotopes (Khokhlov 1989), who suggested that \( ^{12}\text{C} \rightarrow ^3\text{He} \) is the most important one; see the discussion in

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\(^2\) http://cococubed.asu.edu/

\(^3\) http://jinaweb.org/reaclib/db/

\(^4\) https://www.nndc.bnl.gov/ensdf/

\(^5\) The differences are probably because new experimental values became available since the last time \textsc{winvnn\_v2.0\_dat} was updated. (Schatz, private communication).

\(^6\) The file \textsc{isotopes.pfit.dat} is included in the online-only supporting information and is also available through https://www.dropbox.com/sh/f6ys2ce0896lxvvg/AAACd93RR82LyDyY091Eu4u?dl=0

\(^7\) Since again, the differences are probably because new experimental values became available since the last time \textsc{winvnn\_v2.0\_dat} was updated. (Schatz, private communication).

\(^8\) Suggested by Hendrik Schatz.
Sections 5.1.3 and 5.2.2). We, therefore, add to the lists of isotopes obtained from the NSE condition more isotopes, in several stages, which are as follows.

We define an isotope list $\alpha$-ext that describes burning through $\alpha$-elements, which includes:

(i) $n$, $p$ and the $\alpha$-isotopes $^4$He, $^{12}$C, $^{16}$O, $^{20}$Ne, $^{24}$Mg, $^{28}$Si, $^{32}$S, $^{36}$Ar, $^{40}$Ca, $^{44}$Ti, $^{48}$Cr, $^{52}$Fe and $^{56}$Ni.

(ii) All isotopes that differ from $\alpha$-isotopes by $n$, $p$ or $\alpha$.

(iii) $^{22}$Ne, since it has a significant mass fraction for some initial conditions.

(iv) All isotopes of an element between the minimal and the maximal nucleon numbers determined from the previous steps.

(v) We exclude $^5$He and $^9$B from the list, see below.

The obtained $\alpha$-ext list includes 78 isotopes and is presented in Table 1. NSE7 is the combination of all species that meet the $Y_{\text{min}} = 10^{-7}$ threshold and all species from the $\alpha$-ext (actually, the only isotope from $\alpha$-ext that does not meet the $Y_{\text{min}} = 10^{-7}$ threshold is $^{19}$Ne). NSE7 $\alpha$ (y = 4,5,6) is the combination of all species with $Z > 14$ that meet the $Y_{\text{min}} = 10^{-7}$ NSE threshold, those with $Z \leq 14$ that meet the $Y_{\text{min}} = 10^{-7}$ NSE threshold, and all species from the $\alpha$-ext list. The inclusion of all isotopes with $Z \leq 14$ that meet the $Y_{\text{min}} = 10^{-7}$ NSE threshold in NSE4 – 6 only slightly increases the sizes of these nets and improves the calculation of the low-$Z$ isotopes. The obtained lists are presented in Table 1. One can verify that the extended list includes for each element at least one additional isotope with a larger (smaller) nucleon number compared to our most detailed NSE7 list, or that there are no more isotopes with smaller or larger nucleon numbers (bold numbers in Table 1). Furthermore, the extended list contains isotopes of Br and Kr, none of which survive in NSE7. Unless otherwise stated, the NSE7 net is the one used from this point on in the text.

Finally, in order to verify that we are not missing any important low-$Z$ isotopes, we add to the NSE7 list all the isotopes with a $Z \leq 14$ from the extended list that have a measured mass and ground-state spin (not calculated). We call this list NSE7Si and it is presented in Table 1.

The forward reaction rates are taken from JINA (the default library of 2017 October 20). All strong reactions that connect between isotopes from the list are included (this requires some modification of the relevant subroutines of MESA). To allow the plasma to reach an NSE, inverse reaction rates were determined according to a detailed balance. We modified the relevant subroutine of MESA so as to be exactly compatible with Equation (9). Enhancement of the reaction rates due to screening corrections and their compatibility with Equation (9) are described in Section 3.4.

A note is in place regarding the total cross-sections for the reactions $^{12}$C+$^{16}$O and $^{16}$O+$^{16}$O given by JINA. According to JINA, these rates are taken from Caughlan & Fowler (1988, CF88). Caughlan & Fowler (1988) provide the total cross-section for these reactions, as well as the yields of $n$, $p$, and $\alpha$ for these reactions. They note that the sum of these yields can exceed unity because of reactions such as $^{16}$O($^{16}$O,$n$)$^{30}$P and $^{16}$O($^{16}$O,2$p$)$^{30}$Si. This should not be confused with branching ratios for different channels that always sum up to unity. Since the branching ratios are not given by Caughlan & Fowler (1988) for the $^{12}$C+$^{16}$O and $^{16}$O+$^{16}$O reactions, it is not clear how the branching ratios were determined for the $n$, $p$, and $\alpha$ channels provided by JINA for these reactions (other channels, such as $np$ and 2$p$, are not provided).

Therefore, the total cross-sections of $^{12}$C+$^{16}$C (blue), $^{12}$C+$^{16}$O (red) and $^{16}$O+$^{16}$O (black) from the JINA reaclib database (solid lines) and from STARLIB (points) divided by the total cross-sections of Caughlan & Fowler (1988). The ratios for $^{12}$C+$^{16}$O and for $^{16}$O+$^{16}$O are larger by factors that roughly equal the $n$, $p$, and $\alpha$ yields of the reactions (dashed lines, as given by Caughlan & Fowler 1988), which suggest that a choice was made to conserve the yields of $n$, $p$, and $\alpha$ instead of conserving the total cross-section.

![Figure 1](https://starlib.github.io/Rate-Library/)

### 3.3 Equation of state

The EOS is composed of contributions from electron–positron plasma, radiation, ideal gas for the nuclei, Coulomb corrections and nuclear level excitations:

\[
\begin{align*}
\varepsilon &= \varepsilon_{\text{ep}} + \varepsilon_{\text{rad}} + \varepsilon_{\text{ion}} + \varepsilon_{\text{coul}} + \varepsilon_{\text{ex}}, \\
\rho &= \rho_{\text{ep}} + \rho_{\text{rad}} + \rho_{\text{ion}} + \rho_{\text{coul}}, \\
S &= S_{\text{ep}} + S_{\text{rad}} + S_{\text{ion}} + S_{\text{coul}} + S_{\text{ex}}.
\end{align*}
\]

\footnote{\textsuperscript{10} the $^{12}$C($^{16}$O,$n$)$^{27}$Si rate is calculated as the reverse rate of $^{27}$Si,n,$^{12}$C$^{16}$O.}

\footnote{\textsuperscript{11} https://starlib.github.io/Rate-Library/}
Table 1. The lists of isotopes used in this work. Bold numbers mark the minimal or maximal nucleon numbers available in WINV_N2.0.DAT.

| Element | Extended | NSE7Si | NSE7 | NSE6 | NSE5 | NSE4 | α - ext |
|---------|----------|--------|------|------|------|------|---------|
|     | 581 isotopes | 344 isotopes | 260 isotopes | 218 isotopes | 179 isotopes | 137 isotopes | 78 isotopes |
| n | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| H | 1–3 | 1–3 | 1–3 | 1–3 | 1–3 | 1–3 | 1–3 |
| He | 3–4, 6 | 3–4, 6 | 3–4, 6 | 3–4, 6 | 3–4, 6 | 3–4, 6 | 3–4 |
| Li | 6–9 | 6–9 | 6–7 | 6–7 | 6–7 | 6–7 | – |
| Be | 7, 9–13 | 7, 9–13 | 7, 9–10 | 7, 9–10 | 7, 9–10 | 7, 9–10 | – |
| B | 8, 10–14 | 8, 10–14 | 10–11 | 10–11 | 10–11 | 10–11 | 11 |
| C | 9–17 | 9, 11–16 | 11–14 | 11–14 | 11–14 | 11–14 | 11–13 |
| N | 12–20 | 12–19 | 13–15 | 13–15 | 13–15 | 13–15 | 13–15 |
| O | 13–24 | 13–24 | 15–18 | 15–18 | 15–18 | 15–18 | 15–17 |
| F | 14–27 | 14–27 | 17–19 | 17–19 | 17–19 | 17–19 | 17–19 |
| Ne | 17–34 | 17–31 | 19–23 | 19–23 | 19–23 | 19–23 | 19–22 |
| Na | 19–37 | 19–33 | 21–25 | 21–25 | 21–25 | 21–25 | 21–23 |
| Mg | 20–40 | 20–36 | 23–28 | 23–28 | 23–28 | 23–28 | 23–25 |
| Al | 22–43 | 23–35 | 25–30 | 25–30 | 25–30 | 25–30 | 25–27 |
| Si | 23–44 | 24–40 | 27–33 | 27–33 | 27–33 | 27–33 | 27–29 |
| P | 26–40 | 29–35 | 29–34 | 29–34 | 29–33 | 29–31 | 29–31 |
| S | 28–45 | 30–37 | 30–37 | 31–37 | 31–36 | 31–36 | 31–33 |
| Cl | 31–46 | 32–39 | 32–39 | 33–39 | 33–37 | 33–37 | 33–35 |
| Ar | 32–49 | 34–42 | 34–42 | 35–41 | 35–39 | 35–37 | 35–37 |
| Kr | 35–51 | 37–45 | 37–45 | 37–44 | 37–41 | 37–39 | 37–39 |
| Ca | 36–54 | 41–51 | 41–51 | 41–50 | 41–48 | 41–43 | 41–43 |
| Sc | 40–56 | 43–53 | 43–53 | 43–52 | 43–51 | 43–50 | 43–45 |
| Ti | 40–58 | 43–53 | 43–53 | 43–52 | 43–51 | 43–50 | 43–45 |
| V | 42–58 | 45–55 | 45–55 | 45–54 | 45–53 | 45–51 | 45–47 |
| Cr | 44–59 | 47–57 | 47–57 | 47–56 | 47–55 | 47–54 | 47–49 |
| Mn | 46–60 | 49–59 | 49–59 | 49–58 | 49–57 | 49–56 | 49–51 |
| Fe | 48–64 | 50–62 | 50–62 | 51–61 | 51–59 | 51–58 | 51–53 |
| Co | 50–65 | 52–64 | 52–64 | 53–63 | 53–61 | 53–60 | 53–55 |
| Ni | 52–71 | 54–66 | 54–66 | 55–65 | 55–64 | 55–61 | 55–57 |
| Cu | 54–72 | 56–68 | 56–68 | 57–67 | 57–65 | 57–61 | 57 |
| Zn | 56–77 | 58–70 | 58–70 | 59–69 | 60–67 | – | – |
| Ga | 58–78 | 61–72 | 61–72 | 62–70 | – | – | – |
| Ge | 60–82 | 64–74 | 64–74 | 65–71 | – | – | – |
| As | 62–83 | 69–75 | 69–75 | – | – | – | – |
| Se | 64–86 | 75 | 75 | – | – | – | – |
| Br | 70–86 | – | – | – | – | – | – |
| Kr | 71–91 | – | – | – | – | – | – |

We use the Timmes EOS\(^{12}\) (Timmes & Arnett 1999) for the electron–positron plasma and the EOS provided by MESA for the ideal gas part of the nuclei, for the radiation and for the Coulomb corrections (but based on Chabrier & Potekhin (1998) and not on Yakovlev & Shalybkov (1989), see detailed discussion in Section 3.4). We further include the nuclear level excitation energy of the ions and a more accurate expression for the entropy of the ions. As demonstrated in Section 4, the nuclear level excitations can be the most important correction term for an ideal EOS for the relevant thermodynamic states. Although this term was included in Khokhlov (1988) and probably also in Khokhlov (1989, see discussion in Section 5.1.5), it is not part of the EOS routines provided by FLASH (Fryxell et al. 2000) and MESA. In fact, this term is not even mentioned in Fryxell et al. (2000) as a relevant correction for an ideal EOS, who argued that the most important correction is the ion–ion Coulomb interaction term. We show below that nuclear level excitations can be a more important correction to the energy

\(^{12}\) http://cococubed.asu.edu/
than the Coulomb correction (but since nuclear level excitations do not contribute to the pressure, the Coulomb correction is the most important correction to the pressure). We make our EOS publicly available\(^\text{13}\).

An alternative for using the Timmes EOS is using the more efficient Helmholtz EOS (Timmes & Swesty 2000), which is a table interpolation of the Helmholtz free energy as calculated by the Timmes EOS over a density-temperature grid. Although the accuracy of the interpolation is better than \(10^{-7}\) for the relevant density–temperature region with dense enough grid, an internal inconsistency of the Helmholtz EOS precludes obtaining a numerical accuracy of \(10^{-3}\) for our results within some regions of the relevant parameter space. This issue may also be relevant for other applications, and it is discussed in Appendix B.

3.3.1 Nuclear level excitations

The nuclear level excitation energy is given by (Landau & Lifshitz 1980):

\[
\varepsilon_{\text{ex}} = N_A k_B T \sum_i Y_i \frac{\partial \ln w_i(T)}{\partial \ln T} \tag{13}
\]

The nuclear level excitations do not contribute to the pressure, but they do contribute to the entropy:

\[
S_{\text{ex}} = \varepsilon_{\text{ex}} / T. \tag{14}
\]

The input parameters for the EOS routines in MESA are \(\rho, T, \bar{A}\) and \(\bar{Z}\). In order to calculate \(\varepsilon_{\text{ex}}\), the routines must be modified to include \(X_i\) as input parameters. The routines were further modified to supply partial derivatives with respect to \(X_i\), in order to integrate Equations (4).

3.3.2 A more accurate expression for the entropy of the ions

The entropy of the ions (not including the nuclear level excitations) is given by (see e.g. Shapiro & Teukolsky 1983):

\[
S_{\text{ion}} \approx k_B N_A \sum_i \frac{X_i}{\bar{A}_i} \ln \left[ \frac{e^{5/2} (2\pi k_B T)^{3/2}}{\rho \bar{A}_i} \left( \frac{A_i}{N_A} \right)^{5/2} \right]. \tag{15}
\]

This expression can be compared with the one used by MESA:

\[
S_{\text{ion}} = k_B N_A \frac{A}{\bar{A}} \ln \left[ \frac{e^{5/2} (2\pi k_B T)^{3/2}}{\rho} \left( \frac{\bar{A}}{N_A} \right)^{5/2} \right]. \tag{16}
\]

which assumes \(w_i(T) = 1\) and averages in some sense over the mass fractions. This is a reasonable choice in the case that \(X_i\) are not given, but since \(X_i\) are required in order to calculate the nuclear level excitations, we use the more accurate expression for the entropy, Equation (15).

3.4 Coulomb corrections

For the plasma conditions relevant to thermonuclear supernovae, the ion–ion electron interaction, \(Z^2 e^2 (4\pi n_e e/3)^{1/3}\), where \(e\) is the electron charge and \(n_e\) is the electron number density, is weak compared to the kinetic energy of the electrons (\(\lesssim 10\%\) at most). Assuming commutativity of the kinetic and potential operators and the separation of the traces of the electronic and ionic parts of the Hamiltonian, the non-ideal corrections to the plasma due to the Coulomb interaction can be divided into exchange correlation of the electron fluid (electron–electron), ion–electron (polarisation) interaction and ion–ion interaction (see e.g. Chabrier & Potekhin 1998). The relevant conditions for thermonuclear supernovae include both the relativity parameter, \(p_F/m_e c^2\), where \(p_F\) is the zero-temperature Fermi momentum of electrons, and the degeneracy parameter, \(T/T_F\), where \(T_F\) is the Fermi temperature, larger or smaller than unity.

An analytical parameterization of the electron–electron term (exchange and correlation) was given for non-relativistic electrons by Ichimaru et al. (1987) and by Stolzmann & Blöcker (2000). For relativistic electrons, the exchange part was given for high degeneracy by Stolzmann & Blöcker (2000)\(^{14}\) and the full term (exchange and correlation) was given by Janacovici (1962) for zero temperature. As far as we know, there is no available parameterization of the correlation part for relativistic electrons at finite temperatures, nor for the exchange part for relativistic electrons at slight degeneracy, as they are expected to be small. Since these regimes are relevant for thermonuclear supernovae, we inspected the available exchange and correlation terms near these regimes and found them to be a correction smaller than \(0.1\%\). However, we cannot verify that they are on the sub-percent level throughout these regimes. For regimes where a parameterization of the electron–electron term is available, the correction is larger than \(1\%\) only for low densities \(\rho_F \lesssim 0.03\) and low temperatures \(T_F \lesssim 0.2\). We will here-avoid these regions (unless stated otherwise), and, therefore, neglect the electron–electron term, which introduces a sub-percent order of uncertainty. We also neglect the ion–ion term, given for arbitrary degeneracy and relativity of the electrons by Potekhin & Chabrier (2000), as it introduces a correction smaller than \(3 \times 10^{-3}\) for the relevant conditions of thermonuclear supernovae.

The ion–ion interaction term for a plasma with only one type of \(N_i\) ions is given as the dimensionless Helmholtz free energy \(F_i/N_i k_B T \equiv f_i = f_i(\Gamma_i)\), with an ion coupling parameter \(\Gamma_i = Z_i^3 / \bar{Z}_i e \) and an electron coupling parameter \(\Gamma_e = (4 \pi \rho N_i Y_e / 3)^{1/3} e^2 / k_B T\). It is useful to note that \(\Gamma_i \approx 1.1 (T/2 \times 10^8 K)^{-1} (\rho N_i)^{1/3} (10^8 \text{g cm}^{-3})^{1/3} (Z_i^3)^{1/3}\). A useful four-parameter fit for \(f_i(\Gamma)\) was given by Hansen et al. (1977), which is shown in Figure 2. The fit interpolates between the Deyhe–Hückel–Abbe (Abe 1959) result in the weak coupling limit (\(\Gamma \ll 1\)) and the strong coupling limit (\(\Gamma \gg 1\)) that can be simulated. The fit is not valid above the melting point (\(\Gamma \approx 175\)). Later on, Yakovlev & Shalybkov (1989) provided a fit for \(f_i(\Gamma)\) with a different functional form. Their results do not deviate by more than \(1\%\) from the fit of Hansen et al. (1977), but their fit is not continuous at \(\Gamma = 1\); see Figure 2. This is because they required continuity only for \(\Delta f / f \Gamma^2\), but this leads, for example, to a discontinuity in the entropy. The Helmholtz EOS uses the same functional form of Yakovlev & Shalybkov (1989) with somewhat different numerical values, and suffers from the same problem. Chabrier & Potekhin (1998) used the fit of Hansen et al. (1977) with three parameters, and their results do not deviate by more than \(1\%\) from the fit of Hansen et al. (1977). Finally, Potekhin & Chabrier (2000) introduced a seven-parameter fit\(^ {15}\) that deviates from the three-parameter fit of Chabrier & Potekhin

\(^{13}\) Note that their equation (82) is wrong by a minus sign, and their equation (85) should be \(u_{\text{ex}} = f_{\text{ex}}(1 + V_p^b / W_p^b + W_p^b / W_p^b)\).

\(^{14}\) Note that the term \(-B_2 \ln(1 + \Gamma / B_1)\) in their equation (16) should be replaced with \(-B_2 \ln(1 + \Gamma / B_2)\).
(1998) by less than a percent. We hereunder use the fit for \( f(\Gamma) \) of Chabrier & Potekhin (1998), since it is the simplest one and it is accurate to better than a percent.

When the plasma comprises a mixture of different ions, there are situations where the linear mixing rule (LMR), which states that the correction is a number weighted linear sum of one component plasma, is a good approximation (Hansen et al. 1977). If the LMR applies, then the Coulomb correction to the chemical potential of each ion is given by \( \mu_{\text{coul}} = k_B T f_i \) and is independent of the other ions. Nevertheless, at the weak coupling regime the LMR fails, as the Debye–Hückel limit is non-linear. Potekhin et al. (2009a) and Potekhin et al. (2009b) studied the transition to the Debye–Hückel limit and showed that the LMR is accurate to better than 10 percent for \( \Gamma = (Z^5)^3 / \Gamma_c > 1 \), where \( (Z^5)^3 \) is a number weighted sum. The relevant NSE state of the detonation waves are in the regime \( 0.1 \lesssim \Gamma \lesssim 1 \), where the LMR can introduce deviations of up to \( \sim 30\% \). Even larger deviations can be obtained for \( 0.01 \lesssim \Gamma \lesssim 0.1 \), which is typical of the post-shock conditions of helium detonations (although the plasma includes mainly helium ions there). Potekhin et al. (2009b) suggested a modification of \( f_i \) to accurately describe the transition to the Debye–Hückel limit. This modification makes \( \mu_{\text{coul}} \) dependent on other ions in the plasma, which significantly complicates the calculation of the NSE state (Nadyozhin & Yudin 2005). We show later that the Coulomb correction changes the NSE state by a few percent, which means that the modification of the LMR is usually a sub-percent correction (but could be higher). We, therefore, choose in this work to adopt the LMR.

Once the ion–ion terms are determined, the correction of the EOS, the correction of the NSE relation, Equation (9), and the screening of the thermonuclear reaction can be calculated self-consistently. Usually, however, this is not the case. Sometimes only the corrections to the EOS are considered (e.g., as in Khokhlov 1988, 1989), and sometimes all corrections are considered but not in a consistent way (see below). Here we consider all corrections in a consistent way. Following Khokhlov (1988), we approximate the LMR correction to the EOS by \( f(\Gamma) \) for a ‘mean’ nucleus \( \Gamma = \bar{Z}/3\Gamma_c \). This introduces an error of only a few percent compared with LMR (i.e. summing over all ions) and significantly simplifies the calculation of these corrections. For the

NSE relation, we use \( \mu_{\text{coul}} = k_B T f_i \), and this determines, from detailed balance, the screening factors of all thermonuclear reactions (Kushnir & Waxman 2018). In brief, consider the screening of a reaction with reactants \( i = 1, \ldots, N \) with charges \( Z_i \). The screening factor for this reaction is identical to the screening factor of a reaction in which all reactants form a single isootope \( j \) with a charge \( Z_j = \sum_{i=1}^{N} Z_i \) and a photon. The inverse reaction, photodisintegration, is not screened, and, therefore, from the detailed balance condition we get for the screening factor:

\[
\exp \left( \frac{-\sum_{i=1}^{N} \mu_i^C - \mu_j^C}{k_B T} \right)
\]

(same as equation (15) of Dewitt et al. 1973, for the case of \( N = 2 \)). The screening routines available in MESA are not compatible with our choice of \( \mu_i \), and they also include ‘quantum’ corrections (Alastuey & Jancovici 1978). Although these screening factors can still be enforced to satisfy a detailed balance (Calder et al. 2007), we choose to use Equation (17) as it is consistent with our NSE relation and as the ‘quantum’ corrections have a negligible effect on thermonuclear detonation waves. We hereunder refer to both the inclusion of the Coulomb correction terms for the NSE and the screening of thermonuclear reaction as the ‘Coulomb correction term for the NSE state’.

### 4 CJ DETONATIONS

In this section, we calculate several properties of the CJ detonations. This is useful because CJ detonations are independent of reaction rates, which allows an efficient benchmarking for the EOS and the NSE routines. Furthermore, even for initial conditions where the unsupported detonation is pathological, the final CJ NSE conditions provide a good approximation for the pathological NSE conditions. We numerically determined the CJ detonation speed, \( D_{\text{CJ}} \), to an accuracy of \( \sim 10^{-5} \), which allows benchmarking to the accuracy level we aimed for, \( 10^{-3} \). In Section 4.1, we consider the initial composition of CO. We further compare our results to Brenn (1972, Section 4.1.1), Khokhlov (1988, Section 4.1.2) and Gamezo et al. (1999, Section 4.1.3). In Section 4.2, we consider the initial composition of pure helium, and compare our results to Mazurek (1973b, Section 4.2.1) and Khokhlov (1988, Section 4.2.2). We exploit the comparisons to previous works to highlight the sensitivity of the results to various assumptions.

#### 4.1 CJ detonations of carbon-oxygen mixtures

The calculated \( D_{\text{CJ}} \) for CO is presented in the upper panel of Figure 3 for an upstream temperature of \( T_{0,9} = 0.2 \) and an upstream density in the relevant range for supernovae, \( [10^6, 5 \times 10^9] \text{g/cm}^3 \). Similarly to Gamezo et al. (1999) and Dunkley et al. (2013), we find that \( D_{\text{CJ}} \) is not a monotonic function of \( \rho_0 \) and that it has a maximum at \( \rho_{0,7} \approx 0.35 \) and a minimum at \( \rho_{0,7} \approx 4.3 \) (the minimum can also be extracted from table IV of Khokhlov (1988)). Key isotopes at the CJ NSE state are presented in the bottom panel of Figure 3 for the same upstream values. We only present the mass fraction of isotopes that have a mass fraction larger than \( 5 \times 10^{-2} \) at some \( \rho_0 \) within the inspected range. At low densities, the NSE state is dominated by \( ^{56}\text{Ni} \) (with \( \tilde{\rho} \approx 55 \) and \( \tilde{\rho} \approx 56 \) at \( \rho_{0,7} = 0.1 \)), while at higher densities the NSE state is mainly a mixture of \( ^4\text{He}, \ ^{54}\text{Fe}, \ ^{55}\text{Co} \), and \( ^{58}\text{Ni} \) (with \( \tilde{\rho} \approx 12 \) and \( \tilde{\rho} \approx 52 \) at \( \rho_{0,7} = 500 \)). A few key parameters of these CJ detonations are given in Table 2.
The structure of detonation waves

The temperature at the CJ NSE state increases monotonically with the density of the upstream density, and is slightly larger in magnitude than the Coulomb corrections. The contribution of the Coulomb corrections to the initial state is of the order of a few percent (highest contribution in the lowest densities). A slightly smaller contribution is obtained at the NSE state (see Table 2). The Coulomb interaction terms also change the NSE state by a few percent (see Sections 4.1.1 and 4.1.2). We, therefore, estimate the uncertainty of the results to be on the sub-percent level (see Section 3.4).

4.1.1 Comparing CO CJ detonations to Bruenn (1972)

Bruenn (1972) calculated CJ detonations for an initial composition of $X(^{12}\text{C}) = X(^{16}\text{O}) = 0.49$, $X(^{20}\text{Ne}) = 0.02$, an upstream temperature of $T_{0,9} = 0.3$ and a few values of the upstream density in the range of $[5 \times 10^6, 3 \times 10^9]$ g/cm$^3$. We calculated the CJ NSE states for the same initial conditions by following the input physics of Bruenn (1972) as closely as possible. The EOS that was used for the CJ NSE values did not include nuclear-level excitation terms and probably did not include Coulomb terms as well. The list of isotopes included 341 isotopes. When possible, the binding energies are taken from Mattauch et al. (1965) and, for the remaining, the exponential mass formula of Cameron & Elkin (1965) was being used. Actually, the mass formula of Cameron & Elkin (1965) seems to contain possible errors, so we apply a few corrections to it (see Appendix C). We assume that these corrections were applied by Bruenn (1972) as well. Finally, the nuclear partition functions of Clifford & Tayler (1965) were used.

The results of our calculations with the same input physics of Bruenn (1972) are compared to the results of Bruenn (1972) in Table 3 for a few representing upstream densities (compare rows ‘B72 setup’ to rows ‘B72’). The obtained $P_{\text{CJ}}$ and $\rho_{\text{CJ}}$ from our calculations are systematically larger than the results of Bruenn (1972) (by $9 \sim 22\%$ and $7 \sim 20\%$, respectively), while $q_{01,\text{CJ}}$ is systematically lower (by $4 \sim 6\%$). We show below that the reason for this discrepancy is the NSE calculation and not the EOS. But first, let us compare the results obtained with the input physics of Bruenn (1972) to the calculation of the same initial conditions with our default input physics (the row ‘Default’), which highlights the sensitivity of the results to various assumptions. We concentrate on the $q_{01,\text{CJ}}$ values for $\rho_{0,7} = 500$ that shows the largest sensitivity. The value for the input physics of Bruenn (1972) deviates from the default input physics value by $\approx 19\%$. The Coulomb term of the NSE reduces the deviation to $\approx 13\%$ and the Coulomb term of the EOS reduces the deviation even further, to $\approx 9\%$. This demonstrates that the sensitivity of the result to the Coulomb corrections

\[ 16 \text{ In figure 1 of (Bruenn 1972), only 337 isotopes are shown; together with } n, p \text{ and } ^{4}\text{He, one isotope is missing. We assume that } ^{44}\text{S is missing from figure 1 since both } ^{44}\text{S and } ^{45}\text{S are included, so we add it to the list of isotopes.} \]

\[ 17 \text{ Some of the values in Mattauch et al. (1965), p. 13 are not clearly visible in the online scanned version. In these cases, we used the modern values, since the values in this paper are almost identical to the modern ones.} \]
can reach as high as 10 percent. Including the nuclear level excitations terms in the EOS (with the modern values of the partition functions) reduces the deviation to ≈1.6%, demonstrating the importance of these terms. The remaining discrepancy is reduced to ≈0.2% by using the modern values for the partition functions instead of the nuclear partition functions of Clifford & Tayler (1965) for the calculation of the NSE.

We turn now to analyse the reason for the differences between the ‘B72 setup’ and ‘B72’ results. A somewhat simpler case to study is the NSE state at some $\rho$, $T$, and $Y_e$ with the same input physics of Brue"enn (1972), given in Brue"enn (1971). We concentrate on the results with a neutron–proton ratio of 1 ($Y_e \approx 0.5$) from table 1 of Brue"enn (1971). The results of our calculations with the same input physics of Brue"enn (1971) are compared to the results of Brue"enn (1971) in Table 4 (compare rows ‘B71 setup’ to rows ‘B71’). Although our pressure calculations agree with those of Brue"enn (1971) to better than 0.5%, the obtained $\bar{A}$ deviates at high temperatures by 5–10%. If we recalculate the pressure with the $\bar{A}$ values of Brue"enn (1971), this only changes the small contributions of the ions, then the pressures agree to better than 1.5 × 10\(^{-3}\). This result suggests that our EOS is consistent with the EOS used by Brue"enn (1971). However, the different values of $\bar{A}$ demonstrate that the NSE states are different, which lead to different CJ NSE states. As the code that was used to calculate the results of Brue"enn (1971) was lost\(^{18}\), we were unable to identify the cause of this discrepancy.

4.1.2 Comparing CO CJ detonations to Khokhlov (1988)

Khokhlov (1988) calculated CJ detonations for CO, an upstream temperature of $T_{0.9} = 0.2$ and a few values of the upstream density in the range of \([10^7, 5 \times 10^9]\) g/cm\(^3\). We calculated the CJ NSE states for the same initial conditions by following the input physics of Khokhlov (1988). The difference between our Coulomb terms and those used by Khokhlov (1988) is smaller than a percent, and since the Coulomb corrections are a few percent at most, this difference can lead to deviations that are smaller than 10\(^{-3}\). The list of isotopes included 83 isotopes, and we used the modern values of the binding energies and partition functions.

Our comparison of the results of our calculations with the same input physics of Khokhlov (1988) to those of Khokhlov (1988) in Table 5 (i.e., comparison of rows ‘K88 setup’ to rows ‘K88’) reveals large deviations at low densities (up to 13% in $q_{01,CJ}$, for example). We suggest below that the reason for the discrepancy is a possible error in the EOS used by Khokhlov (1988). Before we do so, we compare the results obtained with the input physics of Khokhlov (1988) to the calculation of the same initial conditions with our default input physics (the row ‘Default’). The $q_{01,CJ}$ values for the input physics of Khokhlov (1988) deviate from the default input physics value by 1–6%. The Coulomb term for the NSE reduces the deviation to below 10\(^{-3}\). This once again demonstrates that the sensitivity of the result to the Coulomb corrections is on the order of a few percent.

In order to analyse the reason for the differences between the ‘K88 setup’ and the ‘K88’ results, we calculate the pressure and $q_{01,CJ}$ at the NSE state for the values of $\rho_{CI}$ and $T_{CI}$ as given by Khokhlov (1988). The results of our calculations with the same input physics of Khokhlov (1988) are compared to the results of Khokhlov (1988) in Table 6 (compare rows ‘K88 setup’ to rows ‘K88’). The values of $q_{01,CJ}$ usually deviate by less than ≈2% (only for $\rho_{0.7} = 300$ a deviation of ≈5% is obtained), which suggests that the compositions of the NSE states are similar. However, the deviation in the pressures are large for low densities and reach ≈21% for $\rho_{0.7} = 1$. Since the agreement between the Nadyozhin (1974) electron–positron EOS used by Khokhlov (1988) and the EOS used

\[^{18}\text{Bruenn (private communication).}\]
Table 3. Parameters of CJ detonations for an initial composition of $X(^{12}\text{C}) = X(^{16}\text{O}) = 0.49, X(^{22}\text{Ne}) = 0.02$ and an upstream temperature of $T_{\text{up}} = 0.3$ for a few representing upstream densities. For each upstream density, we present the results of Brünn (1972, B2), the results of our calculations with the same input physics of Brünn (1972, B2 setup), B72 setup with the addition of the Coulomb correction term for the NSE (B72 setup + Coul. NSE), the additional inclusion of the Coulomb correction terms for the EOS (B72 setup + Coul. NSE + Coul. EOS), the additional inclusion of the nuclear level excitations terms in the EOS (using the modern values of the partition functions, B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha}$), and by further using the modern values for the partition functions instead of the nuclear partition functions of Clifford & Taylor (1965) for the calculation of the NSE (B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha} + $ part.). The upper rows for each upstream density are the results with our default input physics.

| $\rho_0$ [g/cm$^3$] | Case | $P_{\text{CJ}}/P_0$ | $\rho_{\text{CJ}}/\rho_0$ | $T_{\text{CJ}}$ [10$^9$ K] | $q_{\text{01. CJ}}$ [10$^{17}$ erg/g] |
|---------------------|------|----------------------|-----------------------------|-----------------------------|---------------------------------|
| $5 \times 10^6$     | Default | 10.23 | 1.727 | 4.472 | 7.290 |
|                    | B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha}$ | 10.23 | 1.726 | 4.473 | 7.299 |
|                    | B72 setup + Coul. NSE + Coul. EOS | 10.22 | 1.725 | 4.471 | 7.293 |
|                    | B72 setup + Coul. NSE + Coul. EOS | 10.22 | 1.724 | 4.472 | 7.292 |
|                    | B72 setup + Coul. NSE | 10.08 | 1.723 | 4.468 | 7.297 |
|                    | B72 setup | 10.08 | 1.726 | 4.467 | 7.271 |
|                    | B72 | 8.058 | 1.411 | 4.265 | 7.720 |
| $2 \times 10^8$     | Default | 2.654 | 1.500 | 7.107 | 3.975 |
|                    | B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha}$ | 2.653 | 1.500 | 7.106 | 3.974 |
|                    | B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha}$ | 2.646 | 1.499 | 7.080 | 3.937 |
|                    | B72 setup + Coul. NSE + Coul. EOS | 2.660 | 1.500 | 7.104 | 3.844 |
|                    | B72 setup + Coul. NSE | 2.633 | 1.498 | 7.113 | 3.800 |
|                    | B72 setup | 2.611 | 1.496 | 7.025 | 3.712 |
|                    | B72 | 2.280 | 1.338 | 6.970 | 3.890 |
| $5 \times 10^9$     | Default | 1.653 | 1.302 | 9.801 | 3.519 |
|                    | B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha}$ | 1.653 | 1.302 | 9.799 | 3.518 |
|                    | B72 setup + Coul. NSE + Coul. EOS + $\varepsilon_{x\alpha}$ | 1.650 | 1.301 | 9.725 | 3.462 |
|                    | B72 setup + Coul. NSE + Coul. EOS | 1.666 | 1.305 | 9.823 | 3.213 |
|                    | B72 setup + Coul. NSE | 1.647 | 1.300 | 9.868 | 3.080 |
|                    | B72 setup | 1.628 | 1.295 | 9.497 | 2.902 |
|                    | B72 | 1.492 | 1.210 | 9.414 | 3.017 |

Table 4. The NSE state for a few values of $\rho, T,$ and $Y_c = 0.5$. For each case, we present the results of Brünn (1971, B71), the results of our calculations with the same input physics of Brünn (1971, B71 setup), and the results of recalculating the pressure with the $\bar{A}$ values of Brünn (1971, B71 setup + B71 $\bar{A}$).

| $\rho$ [g/cm$^3$] | $T$ [10$^9$ K] | Case | $P$ [erg/cm$^3$] | $\bar{A}$ |
|-------------------|----------------|------|----------------|----------|
| $1 \times 10^7$   | 6              | B71 setup | $9.423 \times 10^{24}$ | 6.963 |
|                   |                | B71 setup + B71 $\bar{A}$ | $9.459 \times 10^{24}$ | 6.634 |
|                   |                | B71 | $9.461 \times 10^{24}$ | 6.634 |
| $1 \times 10^8$   | 3              | B71 setup | $2.507 \times 10^{25}$ | 55.93 |
|                   |                | B71 setup + B71 $\bar{A}$ | $2.507 \times 10^{25}$ | 55.98 |
|                   |                | B71 | $2.511 \times 10^{25}$ | 55.98 |
| $1 \times 10^9$   | 7              | B71 setup | $4.972 \times 10^{25}$ | 7.609 |
|                   |                | B71 setup + B71 $\bar{A}$ | $4.980 \times 10^{25}$ | 7.527 |
|                   |                | B71 | $4.983 \times 10^{25}$ | 7.527 |
| $2 \times 10^8$   | 3              | B71 setup | $1.262 \times 10^{27}$ | 55.97 |
|                   |                | B71 setup + B71 $\bar{A}$ | $1.262 \times 10^{27}$ | 55.64 |
|                   |                | B71 | $1.262 \times 10^{27}$ | 55.64 |
| $2 \times 10^9$   | 8              | B71 setup | $1.476 \times 10^{27}$ | 14.41 |
|                   |                | B71 setup + B71 $\bar{A}$ | $1.468 \times 10^{27}$ | 15.69 |
|                   |                | B71 | $1.470 \times 10^{27}$ | 15.69 |
by us is better than 0.1% (Timmes & Arnett 1999), the difference is possibly because of some numerical bug. In fact, the difference between the pressures is almost exactly the radiation pressure (compare rows ‘K88 setup + Coul. NSE’ to rows ‘K88’). We conclude that the reason for the discrepancy is an apparent bug in the EOS used by Khokhlov (1988)\(^{19}\).

### 4.1.3 Comparing CO CJ detonations to Gamezo et al. (1999)

Gamezo et al. (1999) calculated CJ detonations for CO, an upstream temperature of \(T_{0,0} = 0.2\) and a few values of the upstream density in the range of \([3 \times 10^7, 3 \times 10^9]\) g/cm\(^3\). The list of isotopes included 13 \(\alpha\)-nuclei, and Coulomb corrections were probably not included. We calculate the CJ NSE states for the same initial conditions by following the input physics of Gamezo et al. (1999). We use the modern values of the binding energies and partition functions.

\(^{19}\) Khokhlov (1988) claims that the discrepancy between his results and the results of Brue"enn (1972) at low densities is because of the approximate EOS used by Brue"enn (1972), while, in fact, we find that the EOS used by Brue"enn (1972) is accurate and the one used by Khokhlov (1988) may contains an error.

The results of our calculations with the same input physics of Gamezo et al. (1999) are compared to the results of Gamezo et al. (1999) in Figure 4 (compare the black lines to the blue lines) and in Table 7 (compare rows ‘G99 setup’ to rows ‘G99’). The general behaviour of both \(D_{CJ}\) and \(q_{0,1,CJ}\) is similar. Deviations of up to \(\approx 2\%\) are obtained in \(D_{CJ}\) and large deviations are obtained at high densities in \(q_{0,1,CJ}\) (\(\approx 7\%\) for \(\rho_{0,7} = 100\)). Below, we try to analyse the reason for the discrepancy.

First, it is not clear how the CJ values were actually calculated by Gamezo et al. (1999), since they claim to integrate the reaction equations to obtain the CJ values. Besides the fact that this is not required, as the CJ values are independent of reaction rates, it is also not possible for pathological detonations, as the integration hits a sonic point for \(D < D_s\). Let us now concentrate on the \(\rho_{0,7} = 1\) case, where we obtain a similar \(q_{0,1,CJ}\) but a lower \(D_{CJ}\). We find from the upper panel of figure 3 of Gamezo et al. (1999) that \(u_{CJ} \approx 0.68 \times 10^4\) km/s and that \(c_{CJ} \approx 0.75 \times 10^4\) km/s. With these \(u_{CJ}\) and \(D_{CJ}\) figures, we get from Equation (2) that \(\rho_{CJ,7} \approx 1.79\). We can now use our EOS (without the Coulomb correction) to find \(C_{CJ}\) in two ways. For the value of \(c_{CJ}\), we find that \(T_{CJ,9} \approx 5.31\), and for the value of \(c_{CJ} = u_{CJ}\), we find that \(T_{CJ,9} \approx 5.10\). This discrepancy demonstrates that the calculation of Gamezo et al. (1999) is inconsistent (to the level of a few percent).

| \(\rho_0\) [g/cm\(^3\)] | Case                  | \(P_{CJ}/P_0\) | \(\rho_0/\rho_{CJ}\) | \(T_{CJ}\) [10\(^8\) K] | \(q_{0,1,CJ}\) [10\(^5\) erg/g] | \(\gamma_{CJ}\) [10\(^5\) km/s] |
|----------------------|----------------------|----------------|-----------------------|-------------------|-------------------|-------------------|
| \(1 \times 10^7\)    | Default              | 7.668          | 0.5760               | 5.058             | 6.478             | 1.1844            | 1.1545            |
|                      | K88 setup + Coul. NSE| 7.675          | 0.5756               | 5.059             | 6.477             | 1.1843            | 1.1546            |
|                      | K88 setup            | 7.656          | 0.5749               | 5.049             | 6.430             | 1.1810            | 1.1518            |
|                      | K88                  | 7.95           | 0.59                 | 4.73              | 7.10              | 1.23              | 1.19              |
| \(3 \times 10^7\)    | Default              | 4.782          | 0.5973               | 5.866             | 5.197             | 1.1747            | 1.1231            |
|                      | K88 setup + Coul. NSE| 4.782          | 0.5973               | 5.866             | 5.197             | 1.1747            | 1.1232            |
|                      | K88 setup            | 4.756          | 0.5970               | 5.838             | 5.131             | 1.1731            | 1.1190            |
|                      | K88                  | 5.15           | 0.59                 | 5.60              | 5.84              | 1.18              | 1.16              |
| \(1 \times 10^9\)    | Default              | 3.169          | 0.6409               | 6.637             | 4.291             | 1.2230            | 1.1345            |
|                      | K88 setup + Coul. NSE| 3.168          | 0.6412               | 6.637             | 4.292             | 1.2230            | 1.1345            |
|                      | K88 setup            | 3.146          | 0.6415               | 6.578             | 4.214             | 1.2224            | 1.1294            |
|                      | K88                  | 3.33           | 0.63                 | 6.47              | 4.67              | 1.21              | 1.16              |
| \(3 \times 10^9\)    | Default              | 2.434          | 0.6814               | 7.362             | 3.833             | 1.2621            | 1.1933            |
|                      | K88 setup + Coul. NSE| 2.435          | 0.6813               | 7.362             | 3.833             | 1.2621            | 1.1934            |
|                      | K88 setup            | 2.415          | 0.6825               | 7.261             | 3.740             | 1.2617            | 1.1873            |
|                      | K88                  | 2.49           | 0.68                 | 7.18              | 4.02              | 1.25              | 1.21              |
| \(1 \times 10^9\)    | Default              | 1.987          | 0.7219               | 8.265             | 3.578             | 1.2898            | 1.3049            |
|                      | K88 setup + Coul. NSE| 1.987          | 0.7218               | 8.264             | 3.578             | 1.2899            | 1.3051            |
|                      | K88 setup            | 1.970          | 0.7233               | 8.093             | 3.454             | 1.2895            | 1.2974            |
|                      | K88                  | 2.01           | 0.72                 | 8.05              | 3.59              | 1.28              | 1.31              |
| \(3 \times 10^9\)    | Default              | 1.739          | 0.7542               | 9.247             | 3.505             | 1.3055            | 1.4475            |
|                      | K88 setup + Coul. NSE| 1.740          | 0.7541               | 9.246             | 3.505             | 1.3056            | 1.4479            |
|                      | K88 setup            | 1.723          | 0.7566               | 8.972             | 3.338             | 1.3053            | 1.4384            |
|                      | K88                  | 1.75           | 0.75                 | 8.95              | 3.59              | 1.30              | 1.45              |
| \(5 \times 10^9\)    | Default              | 1.654          | 0.7680               | 9.769             | 3.518             | 1.3107            | 1.5273            |
|                      | K88 setup + Coul. NSE| 1.654          | 0.7681               | 9.768             | 3.518             | 1.3108            | 1.5279            |
|                      | K88 setup            | 1.639          | 0.7704               | 9.430             | 3.322             | 1.3106            | 1.5175            |
|                      | K88                  | 1.66           | 0.77                 | 9.45              | 3.35              | 1.30              | 1.53              |
Table 6. The pressure and \( q_{0.1,CJ} \) at the NSE state for the values of \( P_{CJ} \) and \( T_{CJ} \) as given by Khokhlov (1988) for CO. For each case, we present the results of \( \text{K88} \), the results of our calculations with the same input physics of \( \text{K88} \), and the results of recalculating the pressure with twice the radiation pressure (K88 setup + twice \( p_{rad} \)).

| \( \rho_0 \) [g/cm\(^3\)] | Case | \( P_{CJ}/P_{K88} \) | \( q_{0.1,CJ} \) [10\(^{17}\) erg/g] |
|-----------------|-----|-----------------|---------------------|
| 1 \times 10\(^7\) | K88 setup | 6.46 | 7.08 |
| | K88 setup + twice \( p_{rad} \) | 7.95 | 7.10 |
| | \text{K88} | 7.95 | 7.10 |
| 3 \times 10\(^7\) | K88 setup | 4.46 | 5.90 |
| | K88 setup + twice \( p_{rad} \) | 5.08 | |
| | \text{K88} | 5.15 | 5.84 |
| 1 \times 10\(^8\) | K88 setup | 3.14 | 4.64 |
| | K88 setup + twice \( p_{rad} \) | 3.34 | |
| | \text{K88} | 3.33 | 4.67 |
| 3 \times 10\(^8\) | K88 setup | 2.40 | 4.03 |
| | K88 setup + twice \( p_{rad} \) | 2.47 | |
| | \text{K88} | 2.49 | 4.02 |
| 1 \times 10\(^9\) | K88 setup | 1.97 | 3.60 |
| | K88 setup + twice \( p_{rad} \) | 1.99 | |
| | \text{K88} | 2.01 | 3.59 |
| 3 \times 10\(^9\) | K88 setup | 1.74 | 3.41 |
| | K88 setup + twice \( p_{rad} \) | 1.75 | |
| | \text{K88} | 1.75 | 3.59 |
| 5 \times 10\(^9\) | K88 setup | 1.64 | 3.28 |
| | K88 setup + twice \( p_{rad} \) | 1.65 | |
| | \text{K88} | 1.66 | 3.35 |

Table 7. Parameters of CJ detonations for CO and upstream temperature of \( T_{0.9} = 0.2 \) for a few upstream densities. For each upstream density, we present the results of Gamezo et al. (1999, G99), the results of our calculations with the same input physics of Gamezo et al. (1999, G99 setup), the G99 setup with the addition of the Coulomb correction term for the NSE (G99 setup + Coul. NSE), and the additional inclusion of the Coulomb correction term for the EOS (G99 setup + Cou. NSE + Cou. EOS), and also the addition of the nuclear level excitations (G99 setup + Cou. NSE + Cou. EOS + \( \varepsilon_{ex} \)). The upper rows for each upstream density are the results with our default input physics.

| \( \rho_0 \) [g/cm\(^3\)] | Case | \( q_{0.1,CJ} \) [10\(^{17}\) erg/g] | \( D_{CJ} \) [10\(^4\) km/s] |
|-----------------|-----|----------------|---------------------|
| 1 \times 10\(^7\) | Default | 6.478 | 1.155 |
| | G99 setup + Coul. NSE + Cou. EOS + \( \varepsilon_{ex} \) | 7.118 | 1.192 |
| | G99 setup + Coul. NSE + Cou. EOS | 7.113 | 1.191 |
| | G99 setup + Coul. NSE | 7.120 | 1.195 |
| | G99 setup | 7.059 | 1.192 |
| | G99 | 7.03 | 1.21 |
| 1 \times 10\(^8\) | Default | 4.291 | 1.134 |
| | G99 setup + Coul. NSE + Cou. EOS + \( \varepsilon_{ex} \) | 4.467 | 1.151 |
| | G99 setup + Coul. NSE + Cou. EOS | 4.427 | 1.153 |
| | G99 setup + Coul. NSE | 4.396 | 1.154 |
| | G99 setup | 4.290 | 1.146 |
| | G99 | 4.17 | 1.14 |
| 1 \times 10\(^9\) | Default | 3.578 | 1.305 |
| | G99 setup + Coul. NSE + Cou. EOS + \( \varepsilon_{ex} \) | 3.650 | 1.315 |
| | G99 setup + Coul. NSE + Cou. EOS | 3.542 | 1.319 |
| | G99 setup + Coul. NSE | 3.459 | 1.320 |
| | G99 setup | 3.310 | 1.309 |
| | G99 | 3.08 | 1.28 |
Because of these unresolved discrepancies, we did not try to reproduce the results of Gamezo et al. (1999) for the pathological case. We will just mention here that the \( q_{0,1} \) values presented in figure 2 of Gamezo et al. (1999) seem to be inconsistent. Our calculations always yield a \( q_{0,1} < q_{0,1,CJ} \). This is because at higher detonation speeds, the temperature of the NSE state is higher and, therefore, more \(^4\)He nuclei are present, which decreases \( q_{0,1} \). Gamezo et al. (1999) obtained \( q_{0,1} > q_{0,1,CJ} \), which seems to be inconsistent. Moreover, from figure 2 of Gamezo et al. (1999), we can extract \( q_{0,1} \approx 4.70 \times 10^{17} \) erg/cm\(^3\) for \( \rho_0 \approx 10 \), while from the bottom panel of figure 3 of Gamezo et al. (1999) we find that \( q_{0,1} \approx 3.57 \times 10^{17} \) erg/cm\(^3\) for the same \( \rho_0 \).

Let us go back now to Table 7 and compare the results obtained with the input physics of Gamezo et al. (1999) to the calculation with our default input physics (the row ’Default’; compare also the blue and the red lines in Figure 4). The \( q_{0,1,CJ} \) values for the input physics of Gamezo et al. (1999) deviate from the default input physics values by up to \( \approx 9\% \). The Coulomb terms and the nuclear level excitations terms change the values of \( q_{0,1,CJ} \) up to a few percent each. Finally, extending the isotope list to our default list changes the values of \( q_{0,1,CJ} \) by \( \approx 2 \rightarrow 9\% \). The reason for this alteration is that \( \alpha \)-nuclei cannot correctly represent the NSE state, as a significant fraction of the mass can be stored in different isotopes (see bottom panel of Figure 3). This inability is compensated for by artificially increasing the mass fractions of all the elements with a \( Z_i \geq 14 \), especially \(^{56}\)Ni and \(^{56}\)Fe. For this reason, calculations with \( \alpha \)-nuclei are inadequate for the accurate analysis that we aim for in this work.

### 4.2 CJ detonations of pure helium

The calculated \( D_{CJ} \) for He is presented in the upper panel of Figure 5 for an upstream temperature of \( T_{0,9} = 0.2 \) and an upstream density in the relevant range for supernovae of \( [10^4, 10^9] \) g/cm\(^3\). Similarly to Dunkley et al. (2013), we find that \( D_{CJ} \) is not a monotonic function of \( \rho_0 \) and that it has a minimum at \( \rho_{0,7} \approx 4.5 \times 10^{-3} \) and a maximum at \( \rho_{0,7} \approx 0.16 \). There is another minimum at \( \rho_{0,7} \approx 7 \), which can also be extracted from table IV of Khokhlov (1988). Key isotopes at the CJ NSE state are presented in the bottom panel of Figure 5 for the same upstream values. We only present the mass fraction of isotopes that have a mass fraction larger than \( 5 \times 10^{-2} \) at some \( \rho_0 \) within the inspected range.
The structure of detonation waves

Table 8. Key parameters of CJ detonations for He and upstream temperature of \( T_{0,9} = 0.2 \).

| \( \rho_0 \) [g/cm\(^3\)] | \( P_0/\rho_0 \) [MeV/m\(^3\)p\(_0\)] | \( \gamma_0 \) \(^{a}\) | \( D_{CJ} \) \([10^8 \text{km/s}]\) | \( P_{CJ}/\rho_0 \) \([\text{MeV/m}^3\text{p}_0]\) | \( \rho_{CJ}/\rho_0 \) | \( T_{CJ} \) \([10^5 \text{K}]\) | \( \gamma_{CJ} \) \(^{b}\) | \( q_{01,CJ} \) \([\text{MeV/m}^3\text{p}_0]\) | \( \Delta C_{J} \) | \( \Delta C_{I} \) | \( f_{\text{cool}} \) \(^{c}\) | \( f_{\text{es}} \) \(^{d}\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1 \times 10^4   | 0.01373         | 1.5967          | 1.4948          | 1.0459          | 1.7937          | 1.341           | 1.2448          | 1.5803          | 56.00           | 56.00           | -3.2            | -10.5           |
| 3 \times 10^4   | 0.01404         | 1.6178          | 1.4731          | 1.0570          | 1.7804          | 1.689           | 1.2659          | 1.5803          | 56.00           | 56.00           | -3.1            | -8.4            |
| 1 \times 10^5   | 0.01590         | 1.6211          | 1.4776          | 0.9977          | 1.7566          | 2.180           | 1.3006          | 1.5803          | 55.99           | 56.00           | -2.9            | -6.6            |
| 3 \times 10^5   | 0.02075         | 1.6082          | 1.5018          | 1.0222          | 1.7400          | 2.776           | 1.3255          | 1.5797          | 55.77           | 55.98           | -2.7            | -5.3            |
| 1 \times 10^6   | 0.03312         | 1.5718          | 1.5342          | 1.0737          | 1.7346          | 3.653           | 1.3213          | 1.5656          | 50.12           | 55.81           | -2.6            | -4.0            |
| 3 \times 10^6   | 0.05443         | 1.5201          | 1.5251          | 1.1194          | 1.7812          | 4.684           | 1.2203          | 1.4462          | 26.54           | 54.80           | -2.7            | -2.9            |
| 1 \times 10^7   | 0.09261         | 1.4585          | 1.4304          | 1.0650          | 1.8357          | 5.860           | 1.0939          | 1.1083          | 41.44           | 53.75           | -2.9            | -2.3            |
| 3 \times 10^7   | 0.1449          | 1.4116          | 1.3430          | 0.9588          | 1.7614          | 6.753           | 1.1151          | 0.8232          | 7.78            | 53.58           | -2.9            | -2.1            |
| 1 \times 10^8   | 0.2279          | 1.3764          | 1.3269          | 0.9421          | 1.6356          | 7.666           | 1.1932          | 0.6564          | 6.57            | 53.35           | -2.8            | -2.0            |

\(^{a}\) \( \gamma_0 = c_s^2/\rho_0 P_0 \)

\(^{b}\) \( \gamma_{CJ} = \left( \epsilon_{CJ}/P_{CJ} \right)^{\mu} \)

\(^{c}\) \( f_{\text{cool}} = \log_{10} \left( \frac{T_{CJ}}{T_{0,9}} \right) \) at the CJ state

\(^{d}\) \( f_{\text{es}} = \log_{10} \left( \frac{\rho_{CJ}}{\rho_0} \right) \) at the CJ state

\( T_{CJ} \) as given by Mazurek (1973b).

The results of our calculations with the M73 setup are compared to the results of Mazurek (1973b) in Table 10 (compare rows ‘M73 setup’ to rows ‘M73’). In order to calculate the electron–positron terms for M73, we assume that the CJ conditions hold and we use the analytical terms for the radiation and the ions (with the M73 setup values for \( \bar{A} \)). The values of \( q_{01,CJ} \) deviate by less than \( \approx 5\% \), which suggests that the compositions of the NSE states are similar, and the difference between the pressure levels is below \( \approx 1\% \), which suggests that our pressure calculation is consistent with the one used by Mazurek (1973b). Indeed, when we directly compare the electron–positron pressures, the deviation is smaller than 1.5\%, which also suggests that the deviation in \( \bar{A} \) is small. However, the electron–positron energies deviate by up to 33\%, with the largest deviation obtained for \( \rho_{0,7} = 0.1 \). We believe that this is because of inaccuracies in the EOS used by Mazurek (1973b) for the high positron-to-proton ratio, \( n_+/n_p \). Mazurek (1973a) admits that his EOS becomes less accurate in higher \( n_+/n_p \), although the error is estimated to be \( \approx 10\% \) for \( n_+/n_p \approx 10 \), where even for \( \rho_{0,7} = 0.1 \) we only have \( n_+/n_p \approx 0.68 \) (see Table 10). Mazurek (1973a) estimated the level of accuracy of his EOS by comparing it to Table A.4.1 in Appendix A.4 of Cox & Giuli (1968), and he claimed that his results match exactly the results there, except for regions with \( n_+/n_p > 50 \). These results are only three entries with \( n_+/n_p > 50 \) in the tables of Cox & Giuli (1968). We can verify almost directly in the case \( \rho_{0,7} = 1 \) that the results of Mazurek (1973b) are not accurate. This is done by using the following values: \( \rho_{CJ} \), \( \mu_0 = 0.82 \) (\( \mu_0 = 2 \)) and \( T_{CJ} = 5.71 \) as given by Mazurek (1973b) with similar values to the entries \( \eta = 0 \), \( \beta = 0 \) (\( T_{0,9} = 5.93 \)) and \( \rho_0/\mu_e = 9.243 \times 10^6 \) g/cm\(^3\) in the tables of Cox & Giuli (1968). There we find \( \rho_{CJ}/\rho_0 \approx 0.3787 \), which does not seem to change too much for \( \approx 10\% \) changes in \( T \) and \( \rho \). Comparing this to the M73 setup value (\( \approx 0.38 \)) and the M73 value (\( \approx 0.46 \)) suggests that the electron–positron energy terms are not accurately calculated by Mazurek (1973b).

We also compare the results obtained with the M73 setup to the calculation of the same initial conditions but with our default input physics (the row ‘Default’ in Table 9). The \( q_{01,CJ} \) values for the M73 setup deviate from the default input physics value at high densities by up to \( \approx 7\% \). The Coulomb correction term for the NSE

20 The electron–electron term is neglected here, and the correction is in the range of a few percent for \( \rho_{0,7} \lesssim 0.027 \) and \( T_{0,9} = 0.01 \).
reduces the deviation to less than 4%, and the Coulomb correction term for the EOS reduces it further to below 3%.

4.2.2 Comparing He CJ detonations to Khokhlov (1988)

Khokhlov (1988) calculated CJ detonations for He, an upstream temperature of $T_0 = 0.1$ and a few values of the upstream density in the range of $[10^6, 10^9]$ g/cm$^3$. We calculated the CJ NSE states for the same initial conditions by following the input physics of Khokhlov (1988). The results of our calculations with the same input physics of Khokhlov (1988) are compared to the results of Khokhlov (1988) in Table 11 (compare rows ‘K88 setup’ to rows ‘K88’). Large deviations are obtained (up to 15% in $q_{01,CJ}$, for example). We showed in Section 4.1.2 that the EOS used by Khokhlov (1988) apparently contains a numerical bug, to which we attribute the difference between the results. We verified this again by calculating the pressure and $q_{01,CJ}$ at the NSE state for the values of $ρ_{CJ}$ and $T_{CJ}$ as given by Khokhlov (1988). The results of our calculations with the same input physics of Khokhlov (1988) are compared to the results of Khokhlov (1988) in Table 12 (compare rows ‘K88 setup’ to rows ‘K88’). The values of $q_{01,CJ}$ deviate by less than ±1%, which suggests that the compositions of the NSE states are similar. However, the deviation in the pressure levels are large for low densities and reach ±3% for $ρ_{0,7} = 0.1$. Once again, the difference between the pressure levels is almost exactly the radiation pressure (compare rows ‘K88 setup + twice $p_{rad}$’ to rows ‘K88’). We also compare the results obtained with the input physics of Khokhlov (1988) to the calculation of the same initial conditions but with our default input physics (the row ‘Default’ in Table 11). The $q_{01,CJ}$ values for the input physics of Khokhlov (1988) deviate from the default input physics by up to ±3%. The Coulomb correction term for the NSE reduces the deviation to below 2.5 × 10^{-3}.

It is interesting to note that Townsley et al. (2012) calculated the $D_{CJ}$ for He: $ρ_{0,7} = 0.5$, $T_{0,9} = 0.2$, by using the Helmholtz EOS and the 13 α-element network. They claim that their value, 1.54 × 10^{4} km/s, is consistent with the results of Khokhlov (1988), as they interpolate between the entries $ρ_{0,7} = 0.3$ and $ρ_{0,7} = 1$ of Table 11. We verified that this is in fact a coincidence, because the apparent numerical bug in the EOS of Khokhlov (1988) compensates for the difference between the input physics of Townsley et al. (2012) and Khokhlov (1988).

5 THE STRUCTURE OF THE DETONATION WAVE

In this section, we present our calculation of the structure of the (possibly pathological) detonation waves. For a given detonation speed, in which the final state is NSE (and the solution does not cross the sonic point), the end state is known in advance, and is independent of the reaction rates. We use this fact to monitor the numerical accuracy of the integration. Another useful method is to monitor the energy conservation during the integration, which allows us to estimate that our numerical accuracy is better than 10^{-3}. The numerical integration is performed with a fourth-order implicit Rosenbrock method (option RODAS4_SOLVER of MESA) with the parameters rtol = 10^{-7} (relative error tolerance) and atol = 10^{-8} (absolute error tolerance). In Section 5.1, we consider the initial composition of CO, and in Section 5.2, we consider the initial composition of He.

5.1 The structure of the detonation wave in CO

In this section, we present the structure of the detonation wave in CO. In Section 5.1.1, we present an example of the structure of a detonation wave for some specific initial conditions. In Sections 5.1.2 and 5.1.3, we calculate the pathological detonation speed, $D_*$, and the structure of the detonation wave, respectively, as a function of the upstream density. We comment on the uncertainty of the results in Section 5.1.4. Finally, we compare our results to Khokhlov (1989) and Townsley et al. (2016) in Sections 5.1.5 and 5.1.6, respectively.

5.1.1 An example for CO: $ρ_{0,7} = 1$ and $T_{0,9} = 0.2$

We first present in Figure 6, as an example, the structure of a detonation wave as a function of the distance behind the shock, $x$, for CO, $ρ_{0,7} = 1$, $T_{0,9} = 0.2$ and a detonation speed of $D = 1.157 \times 10^4$ km/s ($> D_*= 1.1560 \times 10^4$ km/s for these upstream conditions, see below). Following some induction time, the $^{12}C$ is consumed and its mass fraction reaches 0.05 at $x \approx 1.9$ cm (red point in the lower panel), where $\approx 0.26$ MeV/m is released. This is followed by $^{16}O$ burning, which synthesizes heavier elements, most notably $^{28}Si$. It is convenient to mark the end of this process as the state in which the mass fraction of $^{28}Si$ is maximal ($x \approx 2.1 \times 10^3$ cm, orange point in the lower panel). This burning releases additional $\approx 0.36$ MeV/m. As the carbon and oxygen continue to burn, the number of heavy nuclei decreases ($Y$ decreases), while the average mass number $A$ increases. During this stage only a minute amount of $^4He$ is synthesized, such that $A \lesssim 2 \lesssim 30$, as $^{28}Si$ is maximal.

At this stage, the material is in a state of NSQE. Following the approach of Khokhlov (1989), we monitor this by calculating $δ_{56}(x) - δ_{28}(x)$, where

$$δ_i(x) = \ln \left( X_i(x)/X^*_i(x) \right), \quad (18)$$

$X^*_i(x)$ is calculated according to Eq. (9) with $ρ(x)$, $T(x)$, $X_p(x)$, $X_\alpha(x)$; to simplify the notation, we used $i = 28, 56$ for $^{28}Si$, $^{56}Ni$, respectively. The middle panel shows that $|δ_{56}(x) - δ_{28}(x)| \approx 0.1$ slightly after the point in time when the mass fraction of $^{28}Si$ is at a maximum, and it decreases as the solution approach NSE $|δ_{56}(x) - δ_{28}(x)| \approx 0.01$ at $x \approx 1.7 \times 10^3$ cm (orange point).

The middle panel shows that $Y$ slowly decreases towards the NSE value, and we verified that the decrease is controlled by the inverse triple-$\alpha$ reaction, $^{12}C \rightarrow 3^4He$. During this slow burning, not much energy is released, with the heavy elements approaching $A = 55$, while a significant amount of $^4He$ is synthesized, leaving $A \approx 25$.

The approach to NSE is monitored with $δ_{56}(x)$. The middle panel shows that $|δ_{56}| \approx 0.1$ at $x \approx 2 \times 10^3$ cm. From that position, $|δ_{56}|$ decreases exponentially with an $e$-folding distance of $\delta_{56} \approx 5.5 \times 10^7$ cm. The brown point marks the location where $|δ_{56}| = 10^{-3}$. We stop the integration when $δ_{56} = 10^{-3}$, where

$$δ_{\text{max}} = \max_i (|δ_i|), \quad (19)$$

and we do not go over isotopes with either an $X_i < 10^{-20}$ or an $X^*_i < 10^{-20}$. It should be realized that the NSE state is only approximate, and we do not go over isotopes with either an $X_i < 10^{-20}$ or an $X^*_i < 10^{-20}$. It should be realized that the NSE state is only approximate, and we do not go over isotopes with either an $X_i < 10^{-20}$ or an $X^*_i < 10^{-20}$.
at the right edges of the panels), which are calculated only from the conservation laws, is smaller than $10^{-4}$. This demonstrates the high accuracy of our integration.

We mentioned in Section 3.2 that $^{10}\text{C}$ is not included in the isotope list NSE7Si. This isotope approaches its NSE value through the slow reaction $^{10}\text{C}(\alpha, n)^{13}\text{O}$. While this has a negligible effect on the solution, we would have to integrate it over long time periods in order to make sure that $\delta_{\text{max}} = 10^{-3}$. We, therefore, exclude this isotope. This example demonstrates that the distance needed to reach some prescribed deviation from the NSE state is sensitive to the list of isotopes. This is the reason why we monitor the approach to NSE with $\delta_{\text{5G}}$, which is much less sensitive to the isotope list.

Energy conservation during the integration is monitored by the parameter $\delta_{E}$, which is the deviation of the conserved quantity $E - q + P/\rho + u^2/2$ (Bernoulli’s law) from its initial value. The middle panel shows that the value of $\delta_{E}$ increases towards the NSE and is smaller than $10^{-3}$ at the end of the integration. The loss of accuracy is caused by the detailed balance of fast reactions. The time derivative of the mass fraction of each isotope is a sum over all the reactions that involve that isotope. This sum is actually the difference of forward and backward reactions, which should be equal at a detailed balance state. Consider such a difference between two fast reactions as the solution approaches a detailed balance. The accuracy in which this difference is calculated decreases, since it is the difference between two large numbers with many identical significant digits. For most cases, we are able to maintain a high enough numerical accuracy ($\delta_{E} < 10^{-3}$) up to the time when $\delta_{\text{max}} = 10^{-3}$.

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### Table 9. Parameters of CJ detonations for He and upstream temperature of $T_{0,9} = 0.05$ for a few upstream densities.

| $\rho_0$ [g/cm$^3$] | Case | $P_{\text{CJ}}/P_0$ | $\rho_{\text{CJ}}/\rho_0$ | $T_{\text{CJ}}$ [10$^5$ K] | $q_{\text{H},\text{CJ}}$ [10$^7$ erg/g] | $D_{\text{CJ}}$ [10$^5$ km/s] |
|---------------------|------|---------------------|-------------------------|-----------------------------|---------------------------------|-----------------------------|
| 1 $\times$ 10$^6$   | Default | 37.786              | 1.7385                  | 3.651                       | 14.998                          | 1.5339                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 37.780              | 1.7381                  | 3.651                       | 14.998                          | 1.5340                      |
|                    | M73 setup + Coul. NSE | 37.476              | 1.7379                  | 3.649                       | 14.999                          | 1.5344                      |
|                    | M73 setup | 37.459              | 1.7376                  | 3.649                       | 14.994                          | 1.5342                      |
|                    | M73 | 39.00                | 1.56                    | 3.69                        | 15.01                           | 1.70                        |
| 5 $\times$ 10$^6$   | Default | 17.191              | 1.8145                  | 5.193                       | 12.671                          | 1.4936                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 17.200              | 1.8120                  | 5.194                       | 12.664                          | 1.4953                      |
|                    | M73 setup + Coul. NSE | 17.090              | 1.8115                  | 5.193                       | 12.667                          | 1.4958                      |
|                    | M73 setup | 17.074              | 1.8156                  | 5.190                       | 12.596                          | 1.4931                      |
|                    | M73 | 16.90                | 1.64                    | 5.22                        | 12.95                           | 1.59                        |
| 1 $\times$ 10$^7$   | Default | 11.979              | 1.8387                  | 5.857                       | 10.639                          | 1.4310                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 11.987              | 1.8346                  | 5.860                       | 10.616                          | 1.4335                      |
|                    | M73 setup + Coul. NSE | 11.935              | 1.8367                  | 5.861                       | 10.609                          | 1.4340                      |
|                    | M73 setup | 11.898              | 1.8415                  | 5.849                       | 10.499                          | 1.4293                      |
|                    | M73 | 11.10                | 1.64                    | 5.81                        | 10.84                           | 1.49                        |
| 5 $\times$ 10$^7$   | Default | 5.423               | 1.7101                  | 7.135                       | 7.095                           | 1.3270                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 5.429               | 1.7095                  | 7.145                       | 7.024                           | 1.3298                      |
|                    | M73 setup + Coul. NSE | 5.414               | 1.7097                  | 7.146                       | 7.011                           | 1.3303                      |
|                    | M73 setup | 5.365               | 1.7084                  | 7.096                       | 6.893                           | 1.3235                      |
|                    | M73 | 5.16                 | 1.64                    | 7.07                        | 6.95                            | 1.33                        |
| 1 $\times$ 10$^8$   | Default | 4.206               | 1.6394                  | 7.661                       | 6.327                           | 1.3287                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 4.221               | 1.6394                  | 7.675                       | 6.241                           | 1.3317                      |
|                    | M73 setup + Coul. NSE | 4.198               | 1.6381                  | 7.677                       | 6.226                           | 1.3321                      |
|                    | M73 setup | 4.162               | 1.6374                  | 7.604                       | 6.104                           | 1.3250                      |
|                    | M73 | 4.16                 | 1.63                    | 7.60                        | 6.07                            | 1.33                        |
| 5 $\times$ 10$^8$   | Default | 2.788               | 1.5095                  | 9.017                       | 5.478                           | 1.4210                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 2.802               | 1.5111                  | 9.044                       | 5.344                           | 1.4252                      |
|                    | M73 setup + Coul. NSE | 2.788               | 1.5096                  | 9.048                       | 5.314                           | 1.4257                      |
|                    | M73 setup | 2.761               | 1.5069                  | 8.899                       | 5.177                           | 1.4171                      |
|                    | M73 | 2.75                 | 1.50                    | 8.87                        | 5.16                            | 1.42                        |
| 1 $\times$ 10$^9$   | Default | 2.459               | 1.4652                  | 9.698                       | 5.342                           | 1.4913                      |
|                    | M73 setup + Coul. NSE + Coul. EOS | 2.471               | 1.4663                  | 9.732                       | 5.179                           | 1.4964                      |
|                    | M73 setup + Coul. NSE | 2.460               | 1.4652                  | 9.739                       | 5.140                           | 1.4969                      |
|                    | M73 setup | 2.435               | 1.4621                  | 9.542                       | 4.988                           | 1.4875                      |
|                    | M73 | 2.42                 | 1.46                    | 9.50                        | 4.98                            | 1.49                        |
Table 10. The pressure, $q_{01,CJ}$, the electron–positron pressure and the electron–positron energy at the NSE state for the values of $P_{CJ}$ and $T_{CJ}$ as given by Mazurek (1973b). In order to calculate the electron–positron terms for M73, we assume that the CJ conditions hold and we use the analytical terms for the radiation and the ions (with M73 setup values for A). For each case, we present the results of Mazurek (1973b, M73), and the results of our calculations with the M73 setup. We also present the positron-to-proton ratio, $n_e/n_p$, as calculated for the M73 setup.

| $\rho_0$ [g/cm$^3$] | Case | $P_{CJ}/P_{CJ}^{M73}$ | $q_{01,CJ}$ [$10^{17}$ erg/g] | $P_{e,p,CJ}$ [MeV/m$_p$] | $e_{e,p,CJ}$ [MeV/m$_p$] | $(n_e/n_p)_{CJ}$ |
|----------------------|------|----------------------|-------------------------------|------------------------|-------------------|----------------|
| $1 \times 10^6$      | M73 setup | 38.67 | 14.96 | 0.39 | 1.21 | 6.82 $\times 10^{-1}$ |
|                      | M73   | 39.00 | 15.01 | 0.40 | 0.87 |                  |
| $5 \times 10^6$      | M73 setup | 17.00 | 12.33 | 0.41 | 1.13 | 3.56 $\times 10^{-1}$ |
|                      | M73   | 16.90 | 12.95 | 0.40 | 0.94 |                  |
| $1 \times 10^7$      | M73 setup | 11.13 | 10.45 | 0.38 | 1.00 | 2.02 $\times 10^{-1}$ |
|                      | M73   | 11.10 | 10.84 | 0.38 | 0.90 |                  |
| $5 \times 10^7$      | M73 setup | 5.16  | 6.88  | 0.38 | 0.95 | 2.90 $\times 10^{-2}$ |
|                      | M73   | 5.16  | 6.95  | 0.38 | 0.93 |                  |
| $1 \times 10^8$      | M73 setup | 4.15  | 6.08  | 0.42 | 1.06 | 1.01 $\times 10^{-2}$ |
|                      | M73   | 4.16  | 6.07  | 0.42 | 1.05 |                  |
| $5 \times 10^8$      | M73 setup | 2.74  | 5.26  | 0.58 | 1.53 | 6.81 $\times 10^{-4}$ |
|                      | M73   | 2.75  | 5.16  | 0.58 | 1.53 |                  |
| $1 \times 10^9$      | M73 setup | 2.42  | 5.12  | 0.69 | 1.85 | 1.79 $\times 10^{-4}$ |
|                      | M73   | 2.42  | 4.98  | 0.69 | 1.86 |                  |

Table 11. Parameters of CJ detonations for He and an upstream temperature of $T_{0,\gamma} = 0.1$ for a few upstream densities. For each upstream density, we present the results of Khokhlov (1988, K88), the results of our calculations with the same input physics of Khokhlov (1988, K88 setup), and K88 setup with the addition of the Coulomb correction term to the NSE (K88 setup + Coul. NSE). The upper rows for each upstream density are the results obtained with our default input physics.

| $\rho_0$ [g/cm$^3$] | Case | $P_{CJ}/P_0$ | $\rho_0/\rho_{CJ}$ | $T_{CJ}$ [$10^6$ K] | $q_{01,CJ}$ [$10^{17}$ erg/g] | $\gamma_{CJ}$ | $D_{CJ}$ [$10^5$ km/s] |
|----------------------|------|--------------|---------------------|----------------------|------------------------|--------------|----------------------|
| $1 \times 10^6$      | Default | 35.989 | 0.5759 | 3.651 | 14.997 | 1.3214 | 1.5340 |
|                      | K88 setup + Coul. NSE | 35.996 | 0.5758 | 3.651 | 14.997 | 1.3214 | 1.5340 |
|                      | K88 setup | 36.005 | 0.5756 | 3.652 | 14.993 | 1.3208 | 1.5338 |
|                      | K88   | 36.80 | 0.58  | 3.33 | 15.10 | 1.31 | 1.56 |
| $3 \times 10^6$      | Default | 21.671 | 0.5606 | 4.682 | 13.858 | 1.2204 | 1.5251 |
|                      | K88 setup + Coul. NSE | 21.659 | 0.5609 | 4.682 | 13.860 | 1.2204 | 1.5251 |
|                      | K88 setup | 21.658 | 0.5600 | 4.681 | 13.818 | 1.2175 | 1.5235 |
|                      | K88   | 22.60 | 0.57  | 4.34 | 14.50 | 1.26 | 1.57 |
| $1 \times 10^7$      | Default | 11.815 | 0.5443 | 5.857 | 10.633 | 1.0942 | 1.4308 |
|                      | K88 setup + Coul. NSE | 11.819 | 0.5441 | 5.858 | 10.632 | 1.0944 | 1.4308 |
|                      | K88 setup | 11.769 | 0.5433 | 5.844 | 10.527 | 1.0906 | 1.4262 |
|                      | K88   | 12.80 | 0.55  | 5.56 | 12.00 | 1.14 | 1.50 |
| $3 \times 10^7$      | Default | 6.735 | 0.5668 | 6.751 | 7.906 | 1.1154 | 1.3438 |
|                      | K88 setup + Coul. NSE | 6.733 | 0.5671 | 6.752 | 7.913 | 1.1162 | 1.3441 |
|                      | K88 setup | 6.682 | 0.5670 | 6.716 | 7.791 | 1.1148 | 1.3378 |
|                      | K88   | 7.34  | 0.57  | 6.53 | 9.09 | 1.11 | 1.41 |
| $1 \times 10^8$      | Default | 4.182 | 0.6105 | 7.663 | 6.314 | 1.1933 | 1.3281 |
|                      | K88 setup + Coul. NSE | 4.184 | 0.6106 | 7.668 | 6.325 | 1.1943 | 1.3287 |
|                      | K88 setup | 4.146 | 0.6112 | 7.596 | 6.200 | 1.1942 | 1.3217 |
|                      | K88   | 4.47  | 0.60  | 7.50 | 6.95 | 1.17 | 1.37 |
| $3 \times 10^8$      | Default | 3.097 | 0.6473 | 8.560 | 5.635 | 1.2433 | 1.3795 |
|                      | K88 setup + Coul. NSE | 3.099 | 0.6475 | 8.571 | 5.649 | 1.2438 | 1.3805 |
|                      | K88 setup | 3.071 | 0.6482 | 8.451 | 5.510 | 1.2442 | 1.3727 |
|                      | K88   | 3.15  | 0.65  | 8.37 | 5.93 | 1.23 | 1.40 |
| $1 \times 10^9$      | Default | 2.451 | 0.6831 | 9.700 | 5.326 | 1.2761 | 1.4905 |
|                      | K88 setup + Coul. NSE | 2.454 | 0.6828 | 9.717 | 5.340 | 1.2764 | 1.4917 |
|                      | K88 setup | 2.431 | 0.6842 | 9.522 | 5.171 | 1.2771 | 1.4827 |
|                      | K88   | 2.48  | 0.68  | 9.50 | 5.28 | 1.27 | 1.50 |
This is enough to fully describe the approach to NSE, since at this stage all the solution parameters are approaching their NSE values exponentially, at an \( \epsilon \)-folding distance of \( \delta_{\text{NSE}} \). However, for a few cases we were unable to maintain the high accuracy up to the time when \( \delta_{\text{max}} \approx 10^{-3} \). It may be possible to find a specialized algorithm to calculate accurately the approach to NSE, but this is outside the scope of this paper (performing the sums in extended precision is a possibility, see Paxton et al. 2015).

At a distance of \( x \approx 2.0 \times 10^{7} \) cm, the heat release becomes endothermic. This is connected with the minimum of the density \( (\rho = 0 \text{ in Equations (4)}) \) at \( x \approx 2.2 \times 10^{7} \) cm and with the fact that the detonation speed of this solution is slightly above \( D_{s} \). For a detonation speed that equals \( D_{s} \), the position of the point where \( \phi = 0 \) coincides with the sonic point \( (u = c_{s}) \). We numerically determine \( D_{s} \) as the detonation speed for which integration with \( D < D_{s} \) hits the sonic point, \( |u^{2} - c_{s}^{2}|/u^{2} < 10^{-3} \), while integration with \( D > D_{s} \) reaches \( \delta_{\text{max}} = 10^{-3} \). We estimate that these choices limit the numerical accuracy in the determination of \( D_{s} \) to \( \approx 10^{-3} \), since the order of magnitude of error in all terms of Equations (4) should be similar. The sonic point location was determined as the sonic point of the integration with the highest detonation speed that is still smaller than \( D_{s} \). However, because of the rapid change of the sonic point location as \( D \) approaches \( D_{s} \) (Sharpe 1999), the numerical accuracy of the sonic point location is of the order of a few tens of percent. Other properties of the pathological detonation, which are far from the sonic point, are determined to a numerical accuracy that is similar to the numerical accuracy of \( D_{s} \) determination, i.e. \( \approx 10^{-3} \).

### Table 12

The pressure and \( q_{01,CJ} \) at the NSE state for the values of \( P_{CJ} \) and \( T_{CJ} \) as given by Khokhlov (1988) for He. For each case, we present the results of Khokhlov (1988, K88), the results of our calculations with the same input physics of Khokhlov (1988, K88 setup), and the results of recalculating the pressure with twice the radiation pressure (K88 setup + twice \( P_{rad} \)).

| \( \rho_{0} \) [g/cm\(^3\)] | Case | \( P_{CJ}/P_{K88} \) | \( q_{01,CJ} \) [10\(^7\) erg/g] |
|-----------------|---------|-----------------|-----------------|
| 1 \times 10\(^6\) | K88 setup | 25.31 | 15.09 |
| 1 \times 10\(^6\) | K88 setup + twice \( P_{rad} \) | 36.19 | 15.10 |
| 1 \times 10\(^6\) | K88 | 36.40 | 15.10 |
| 3 \times 10\(^6\) | K88 setup | 16.51 | 14.53 |
| 3 \times 10\(^6\) | K88 setup + twice \( P_{rad} \) | 22.56 | 14.50 |
| 3 \times 10\(^6\) | K88 | 22.60 | 14.50 |
| 1 \times 10\(^7\) | K88 setup | 10.02 | 12.00 |
| 1 \times 10\(^7\) | K88 setup + twice \( P_{rad} \) | 12.81 | 12.00 |
| 1 \times 10\(^7\) | K88 | 12.80 | 12.00 |
| 3 \times 10\(^7\) | K88 setup | 6.20 | 9.05 |
| 3 \times 10\(^7\) | K88 setup + twice \( P_{rad} \) | 7.32 | 9.09 |
| 3 \times 10\(^7\) | K88 | 7.34 | 9.09 |
| 1 \times 10\(^8\) | K88 setup | 4.11 | 6.88 |
| 1 \times 10\(^8\) | K88 setup + twice \( P_{rad} \) | 4.48 | 6.95 |
| 1 \times 10\(^8\) | K88 | 4.47 | 6.95 |
| 3 \times 10\(^8\) | K88 setup | 3.02 | 5.94 |
| 3 \times 10\(^8\) | K88 setup + twice \( P_{rad} \) | 3.14 | 5.93 |
| 3 \times 10\(^8\) | K88 | 3.15 | 5.93 |
| 1 \times 10\(^9\) | K88 setup | 2.44 | 5.30 |
| 1 \times 10\(^9\) | K88 setup + twice \( P_{rad} \) | 2.48 | 5.28 |
| 1 \times 10\(^9\) | K88 | 2.48 | 5.28 |

#### 5.1.2 The dependence of \( D_{s} \) on the upstream density

The calculated \( D_{s} \) for CO is presented in the upper panel of Figure 3 for an upstream temperature of \( T_{0,9} \approx 0.2 \). The deviation between \( D_{CJ} \) and \( D_{s} \) is always smaller than \( \approx 1.4\% \) (blue line). We are unable to integrate for densities above \( \rho_{0,7} \approx 340 \) with a high enough accuracy, i.e., \( \delta_{E} < 10^{-3} \). Furthermore, at these high densities, the deviation between \( D_{CJ} \) and \( D_{s} \) approaches our numerical accuracy for \( D_{s} \). Nevertheless, the decrease in the deviation as a function of the upstream density is smaller than exponential, which suggests that even at larger upstream densities the detonation remains pathological. At low densities, the deviation between \( D_{CJ} \) and \( D_{s} \) approaches \( 10^{-3} \) at \( \rho_{0,7} \approx 0.9 \). Nevertheless, we present our results even at lower densities, \( \rho_{0,7} \geq 0.47 \), as long as we were able to integrate with high accuracy. Figure 7 shows that the deviation between \( D_{CJ} \) and \( D_{s} \) decreases exponentially with \( 1/\rho_{0} \), which suggests that the detonation remains pathological even at lower upstream densities. There could be a change in this behaviour at lower densities (maybe connected with the maximum of \( D_{CJ} \) at \( \rho_{0,7} \approx 0.35 \), but we are unable to find evidence for CJ detonations at low upstream densities.

The claim that at low upstream densities, \( \rho_{0,7} \lesssim 1 \), the detonation is CJ was made by Imshennik & Khokhlov (1984) for a pure \(^{12}\)C initial composition and an upstream temperature of \( T_{0,9} \approx 0.2 \). Their claim is based on inspecting whether \( q(x) \) monotonically increases during CJ detonations. However, it is not clear at which point they stopped the integration, and whether the accuracy of the integration is sufficient for meaningful results close to the NSE state. We find that in order to determine the position at which
Figure 6. The structure of an overdriven detonation wave as a function of the distance behind the shock. Upper panel: temperature (blue), density (red), pressure (black) and thermonuclear energy release (green). Middle panel: A (blue), $\bar{A}$ (red), $\delta_{56}$ (see the text, brown), $\delta_{56}(x) - \delta_{56}(x_0)$ (which monitors the NSQE state, orange) and $\delta_F$ (which monitors energy conservation, black). The orange point marks the location where $|\delta_{56} - \delta_{56}(x)| = 10^{-3}$, and the brown point marks the location where $|\delta_{56}(x) - \delta_{56}(x_0)| = 10^{-3}$. Bottom panel: mass fractions of a few key isotopes. The red (orange) point marks the location where the mass fraction of $^{12}\text{C}$ ($^{28}\text{Si}$) reaches 0.05 (is maximal). The points at the right edges of the panels represent the NSE values. At a distance of $x = 2.0 \times 10^7 \text{cm}$, the heat release becomes endothermic. This is connected with the minimum of the density at $x = 2.2 \times 10^7 \text{cm}$.

$q(x)$ begins to decrease, higher and higher numerical accuracy is required for lower and lower upstream densities. This is demonstrated in Figure 7, which shows that the difference between the maximal value of $q$ along the integration and $q_{\text{01}}$ at the end of the integration, $\Delta q$, normalized by $q_{\text{01}}$, decreases exponentially with $1/\rho_0$. It is, therefore, likely that the numerical accuracy of Imshenik & Khokhlov (1984) did not reach the level needed to identify the point at which $q(x)$ begins to decrease for $\rho_{0,7} \lesssim 1$. Sharpe (1999) states that he finds CO detonations to be CJ-type below about $\rho_{0,7} < 2$, but do not explore these densities in detail, constraining the study to higher densities at which the pathological nature is more clear. Gamezo et al. (1999) claim that for CO the detonation is CJ at low densities, based on inspecting whether the flow hits a sonic point and is subsonic downstream and upstream of that point. From their demonstration of this method (bottom panel of their figure 3), it is clear that in their integration they actually did not hit the sonic point, as $u$ deviates from $c_s$ by $\approx 1.5\%$. This procedure depends on numerical accuracy as well, and it seems that Gamezo et al. (1999) did not have the required numerical accuracy to detect pathological detonations at low densities (compare their 1.5% accuracy with the red line in Figure 7).

A few key parameters of these pathological detonations are given in Table 2 for $T_{0,9} = 0.2$. The results are similar to the CJ results, demonstrating that the final CJ NSE conditions provide a good approximation of the pathological NSE conditions.

Similarly to the CJ case, these results do not depend much on the initial upstream temperature. For $T_{0,9} = 0.04$, we are able to integrate within the same range of upstream densities with high enough accuracy. Within this range, the $D_*$ values for $T_{0,9} = 0.04$ deviate from the results for $T_{0,9} = 0.2$ by less than $8 \times 10^{-4}$, and the key parameters of Table 2 deviate by less than $\approx 0.6\%$, with the largest deviation obtained for $q_{\text{01}}$ at $\rho_{0,7} = 300$.
The results calculated with the NSE4 (NSE5) isotope list deviate from the results presented above by less than $7.6 \times 10^{-3}$ ($1.2 \times 10^{-3}$), which suggests that our isotope list is converged to at least $\sim 10^{-3}$. For a given upstream density, the uncertainty of the results is similar to the CJ case (dominated by the uncertainty of the Coulomb correction terms for the EOS and the Coulomb correction terms for the NSE state), and we estimate it to be on the sub-percent level (see detailed discussion in Section 3.4). However, the values of $D_\delta$ itself depend also on the reaction rates and are influenced by uncertainties in these rates. The study of this uncertainty is beyond the scope of this paper, but because of the slight deviation ($\lesssim 1.4\%$) of $D_\delta$ from $D_{CJ}$ (that does not depend on the reaction rates), we speculate that this uncertainty is smaller than a few percent.

5.1.3 The dependence of the burning scales on the upstream density for CO

In Figure 8, different scales of the CO pathological detonation are compared with a typical dynamical scale of $\nu/\sqrt{4\rho_0 v}$ with $V = 10^4\text{ km/s}$. All scales, except for the sonic point location, are determined from the profiles with the lowest detonation speed that is still larger than $D_\delta$ (slightly overdriven). For low densities, $\rho_{0c}/\rho_0 \lesssim 0.47$, where we are unable to determine $D_\delta$, we estimate the scales by integrating with $D = D_{CJ}$. Since at these densities $D_\delta$ (if exists) probably deviates from $D_{CJ}$ by less than $10^{-4}$ and we are able to integrate with high accuracy up to the presented scales, our results should be an excellent estimate. The location where $|\delta S_5| = 10^{-3}$ and $\delta S_0$ are shown as well, which allows to estimate the position of a smaller deviation from NSE. Note that many works present a finite position for NSE that does not have a clear meaning (Kokhlov 1989; Townsley et al. 2016; Dunkley et al. 2013), since the NSE is only obtained asymptotically at infinity. The numerical accuracy of all the scales in Figure 8 is $\lesssim 10^{-3}$, except for the sonic point location with a numerical accuracy of the order of a few tens of percent (see discussion above), which is also the reason for the noisy appearance of this curve.

The ordering of the different scales as a function of the upstream density is similar to the case $\rho_{0c}/\rho_0 = 1$, described in detail in Section 5.1.1. Following some induction time, the $12C$ is consumed and $\rho_{0c} M_{V}/\rho_0$ are released. This is followed by $^{16}O$ burning that synthesizes heavier elements, $\hat{\rho} \approx 30$, roughly when the mass fraction of $^{28}Si$ is maximal. Slightly later, the material is in NSQE ($|\delta S_6 - \delta S_5| = 0.01$), and it approaches NSE while heavier elements are synthesized with $\hat{\rho} \gtrsim 50$ without releasing much energy.

In order to determine which reactions control the approach to NSE (where $\hat{\rho}$ approaches its NSE value), we inspect at the location where $|\delta S_6 - \delta S_5| = 10^{-2}$ and at the location where $|\delta S_5| = 10^{-3}$ the all the reactions that can change the value of $\hat{\rho}$. Of those reactions, the ones that are not in a detailed balance with their reverse reactions dominate the net change in $\hat{\rho}$, so we sort the reactions according to the absolute value of the difference between them and their reverse reactions. The reactions with the largest differences, which control the approach to NSE, are shown in Figure 9. The approach to NSE at the location where $|\delta S_6| = 10^{-2}$ is controlled at low upstream densities, $\rho_{0c}/\rho_0 \lesssim 10$, by the inverse triple-$\alpha$ reaction, $^{12}C + ^{4}He \rightarrow ^{3}He$, and to some extent by $^{3}He + ^{4}He$ reaction, while at high densities, $^{3}He + ^{4}He + ^{3}He$ is the dominant process with an additional contribution from $^{11}B + ^{4}He$ at very high densities, $\rho_{0c}/\rho_0 \gtrsim 200$, $^{11}B + ^{4}He \rightarrow ^{3}He + ^{4}He$ are dominant and comparable. Earlier in the process, where $|\delta S_6 - \delta S_8| = 10^{-2}$, the reactions $^{12}C + ^{4}He \rightarrow ^{4}He + ^{20}Ne$ and $^{12}C + ^{4}He \rightarrow ^{4}He + ^{20}Ne$ are important as well. Except for the inverse triple-$\alpha$ reaction that was known to determine the length-scale of the detonation wave at low densities, the importance of the other reactions was not identified in the past.

The scales themselves shorten significantly as the upstream density increases, due to the increase in the post-shock temperature. Furthermore, the temperature at the NSE state increases monotonically with $\rho_{0c}$, which decreases both $\hat{\rho}$ and $q_{01}$ at these states (see Table 2). At large upstream densities, the released energy is not much larger than the contribution from carbon burning. Usually the detonated material will later cool and $^{4}He$ will recombine to release more energy without a large change in $\hat{\rho}$. The upstream densities in which some values of $q_{01}$ are obtained at the NSE state are marked with dashed lines at the bottom panel of Figure 8. Note that for CJ detonations the scale at which these $q_{01}$ values are obtained should diverge as the upstream density decreases. However, since for pathological detonations the energy release is not monotonic, these $q_{01}$ values are obtained after a finite distance behind the shock wave. Figure 8 allows to estimate for a given upstream density and physical scale the amount of guaranteed energy release and the obtained value of $\hat{\rho}$ (for example, whether iron group elements can be synthesized).

The sonic point location is always above the locations where the mass fraction of $^{28}Si$ is maximal and where $\hat{\rho} \approx 30$. This observation differs from the claims of Gamezo et al. (1999).

A discontinuous behaviour of the sonic point location, from $x \sim 100\text{ cm}$ to $x \sim 10^3\text{ cm}$ around $\rho_{0c}/\rho_0 \approx 2.7$, is seen in the bottom panel of Figure 8 (it was observed by Dunkley et al. (2013) but assumed, without investigation, to be related to the transition between CJ and pathological behavior based on the previous work of Gamezo et al. (1999). There is also a hint for this transition in figure 1 of Townsley et al. (2016)). This is also seen as a minimum of $D_\delta$ at this upstream density in the upper panel of Figure 3. The reason for this behaviour is explained in Figure 10, which shows the slightly overdriven density profiles for $\rho_{0c}/\rho_0 = 0.2$ and an upstream density in the range of $[2.5, 2.9] \times 10^3\text{ g/cm}^3$. For the low upstream densities, there are three locations where $\phi = 0$ (x1, x2, and x3). Each of those points is an extremum point of the density (there is another such point at infinity). The sonic point location for these upstream densities is near $x_3 \sim 10^3\text{ cm}$. As the upstream density increases, there remains only a single location where $\phi = 0$, which is close to $x_1 \sim 10^2\text{ cm}$. Around this transition, the sonic point changes location to $x_1$. We mark this transition as $\phi = 0$, $3 \rightarrow 1$ in the upper panels of Figures 3 and 8. The slight jittering of the sonic point location as the density changes is a consequence of the rapid shift in the sonic point location as $D_\delta$ approaches $D_{CJ}$.

Our analysis indicates some minor dependence of the scales on the upstream temperature (see dotted lines in Figure 11). The largest one is for the carbon-burning scale at high densities. The carbon-burning scale is shown as a function of the upstream temperature in Figure 12 for $\rho_{0c}/\rho_0 = 300$. The burning scale decreases as the upstream temperature increases. This is because the post-shock temperature, $T_{\rho}$, depends slightly on the upstream temperature. This effect is obtained at high densities, where the post-shock plasma is slightly degenerate, making the temperature a sensitive function of the pressure. We note that the ion coupling parameter, $\Gamma$, of the upstream plasma is larger than 200 for $\rho_{0c}/\rho_0 \lesssim 0.032$, where the fit for $\Gamma$ (1) is not valid. This is the reason that we choose $T_{\rho,0} = 0.04\text{ for the temperature sensitivity tests in the previous CO sections.}$
Figure 8. Different scales of the CO pathological detonation in comparison with a typical dynamical scale of \(\sqrt{VG/\rho}\) with \(v = 10^7\) km/s (orange). Top panel: the \(^{12}\text{C}\) consumption scale (blue), \(^{28}\text{Si}\) maximum (red), the location where \(\delta = 0\), \(30\), \(40\), and \(50\) (bottom to top, black), the location where \(|\delta - \delta_{=28}| = 10^{-2}\) (magenta), and the location where \(|\delta - \delta_{=40}| = 10^{-3}\) (green) and \(\delta_{=56}\) (brown). Bottom panel: the locations where the energy release is 0.1, 0.2, ..., 0.7 MeV/m, (bottom to top, black). These scales are determined from the profiles with the lowest detonation speed that is still larger than \(D_s\) (slightly overdriven). The sonic point location (grey, top panel) is determined from the profiles with the highest detonation speed that is still lower than \(D_s\). For low densities, \(\rho_{0,7} \lesssim 0.47\) (indicated by points), where we are unable to determine \(D_s\), we estimate the position of the scales (except the location of the sonic point, \(|\delta_{=56}| = 10^{-3}\) and \(\delta_{=56}\)) by integrating with \(D = D_{CJ}\). Dashed lines in the bottom panel mark the upstream densities at which \(q_{=1}\) obtained at the NSE state matches the indicated energy release. A discontinuous behaviour of the sonic point location, from \(x \sim 100\) cm to \(x \sim 10^4\) cm, is obtained around \(\rho_{0,7} = 2.7\).

5.1.4 The uncertainty of the CO results

The deviations of the positions where \(^{28}\text{Si}\) is maximal and where \(|\delta_{=56}| = 10^{-3}\), calculated with the NSE4, NSE5 and NSE6 isotope lists, from the results calculated with the NSE7 isotope list are presented in Figure 13. Deviations as high as \(\approx 30\%\) are obtained for NSE4, while the deviations of NSE5 and NSE6 are smaller than the percent level. The other scales shown in Figure 8 have smaller deviations. We verified that the deviations of the results obtained with the NSE7Si list deviate by less than a percent from the results obtained with the NSE7 list. This suggests that our calculation of the length-scales is converged to the percent level. The effect of the Coulomb correction is examined in Figure 11. The Coulomb corrections to the EOS are only important at high densities, and they change at most the carbon-burning scale by a factor of \(\sim 2\). The Coulomb correction terms to the NSE have a significant effect at high densities, where they can decrease the length-scales by up to...
one order of magnitude, as they increase the reaction rates. Uncertainty in the reaction rates can be at the same level or even higher, making the length-scales uncertain to a factor of a few. However, a detailed study of the sensitivity to uncertainty in the reaction rates is beyond the scope of this paper.

Figure 11. The ratio between the carbon-burning scale (blue), the positions where $^{28}\text{Si}$ is maximal (red) and where $|\delta_{06}| = 10^{-3}$ (green) obtained under various assumptions and these scales obtained with our default input physics and $T_{0.9} = 0.2$. The solid lines are without the addition of the Coulomb correction term to the EOS, dashed lines are without the addition of the Coulomb correction term to the NSE state and the dotted lines are for $T_{0.9} = 0.04$. For low densities, $\rho_{0.7} \lesssim 0.47$ (left to the black dashed line), we integrated with $D = D_{\text{CJ}}$.

Figure 12. The carbon-burning scale (blue) and the post-shock temperature (red) as a function of the upstream temperature for CO and $\rho_{0.7} = 300$. The ion coupling parameter, $\Gamma$, of the upstream plasma is larger than 200 for $T_{0.9} \lesssim 0.032$ (left to the black dashed line), where the fit for $f(\Gamma)$ is not valid.

\[ \Gamma > 200 \]

\[ \begin{align*}
\rho_0 [\text{g/cm}^3] & \quad 10^0 \\
X^{(12)\text{C}} = 0.05 \quad \text{No Coul. NSE} & \quad 10^1 \\
\text{No Coul. EOS} & \quad 10^2 \\
T_{0.9} = 0.04 & \quad 10^3 \\
\text{28Si maximum, No Coul. NSE} & \quad 10^4 \\
\text{No Coul. EOS} & \quad 10^5 \\
|\delta_{06}| = 10^{-3}, \text{No Coul. NSE} & \quad 10^6 \\
\text{No Coul. EOS} & \quad 10^7 \\
T_{0.9} = 0.04 & \quad 10^8 \\
\end{align*} \]

\[ \rho_0 [\text{g/cm}^3] \quad 10^0 \]

\[ \begin{align*}
X^{(12)\text{C}} = 0.05 \quad [10^{-3}\text{cm}] & \quad 10^0 \\
T_{0.9} & \quad 10^1 \\
\end{align*} \]

\[ \begin{align*}
\Gamma > 200 & \quad 10^0 \\
\rho_0 [\text{g/cm}^3] & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
T_0 [\text{K}] & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
\Gamma > 200 & \quad 10^0 \\
\rho_0 [\text{g/cm}^3] & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
T_{0.9} & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\end{align*} \]

\[ \begin{align*}
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\text{CO, } T_{0.9} = 0.2 & \quad 10^0 \\
\end{align*} \]

Figure 13. The deviations of the positions where $^{28}\text{Si}$ is maximal (red) and where $|\delta_{06}| = 10^{-3}$ (green), calculated with the NSE4 (dotted lines), NSE5 (dashed lines) and NSE6 (solid lines) isotope lists, from the results calculated with the NSE7 isotope list, for CO at $T_{0.9} = 0.2$ as a function of the upstream density. For low densities, $\rho_{0.7} \lesssim 0.47$ (left to the black dashed line), we integrated with $D = D_{\text{CJ}}$.

5.1.5 Comparing the detonation wave structure in CO to Khokhlov (1989)

Khokhlov (1989) calculated the detonation wave structure for CO, an upstream temperature of $T_{0.9} = 0.2$ and a few values of the upstream density in the range of $[10^7, 3 \times 10^9]$ g/cm$^3$. The EOS used by Khokhlov (1989) is the same as the EOS used by Khokhlov (1988)\footnote{Although the nuclear level excitations are missing from the description of the EOS in Khokhlov (1989).}. Since Khokhlov (1989) does not mention the apparent numerical bug in the EOS used by Khokhlov (1988), as we showed in Section 4.1.2, and is citing the same $D_{\text{CJ}}$ values from Khokhlov (1988), we assume that the EOS used by Khokhlov (1989) suffers from the same shortcomings as the EOS used by Khokhlov (1988). The list of isotopes included 114 isotopes, and we used the modern values of the binding energies and partition functions.

We concentrate on the $\rho_{0.7} = 30$, for which Khokhlov (1989) provides detailed results. Khokhlov (1989) reports that $D_s = 1.218 \times 10^4$ km/s, while we find that $D_s = 1.2107 \times 10^4$ km/s for the same input physics (similar deviation was found in Section 4.1.2 for $D_{\text{CJ}}$). It is apparent from our comparison of the structure of an over-driven detonation with $D = 1.233 \times 10^4$ km/s (Figure 14, note the different units of the x-axes of the two panels) that the NSE state is different between the two calculations (especially in the upper panel). This difference is similar in magnitude to the one we found in Section 4.1.2 for the CJ state, suggesting that it is connected with the apparent numerical bug in the EOS used by Khokhlov (1989). This could also be the reason for the higher (lower) temperatures (pressures) that we get around 1 mm. For the $\delta_{\text{NSE}}$, it seems that Khokhlov (1989) plotted $\delta_{38} - \delta_{06}$ (not $\delta_{38} - \delta_{28}$, as claimed by Khokhlov (1989)), so we plot this as well. Note that the scale of $\delta_{\text{NSE}}$ and $\delta_{\text{NSQE}}$ is linear. The abundance of the isotopes, shown in the bottom panel of Figure 14, is similar in the two calculations, except for the much faster consumption of $^{16}\text{O}$ around 1 mm in...
Figure 14. Figures 7 and 8 from Khokhlov (1989). The structure of an overdriven detonation wave for CO, $T_{0,9} = 0.2$, $\rho_{0,7} = 30$ and $D = 1.233 \times 10^4$ km/s, as a function of the distance behind the shock. Black lines are the results of Khokhlov (1989), while the coloured lines are our results with the input physics of Khokhlov (1989). Here, $\delta_{\text{NSE}} = \delta_{56} - \delta_{28}$ (but we actually plot $\delta_{56} - \delta_{28}$, since it seems that Khokhlov (1989) plotted this as well) and $\delta_{\text{NSE}} = \delta_{56}$. The green dashed line in the bottom panel is $A$ (note that the right y-axis label, $A$, is probably a typo, and should be $\langle A \rangle$ with the definitions of Khokhlov 1989). Note that the x-axes units in the two panels are different.

Figure 15. The structure of an overdriven detonation wave for CO, $T_{0,9} = 0.2$, $\rho_{0,7} = 30$ and $D = 1.233 \times 10^4$ km/s, as a function of the distance behind the shock. We show the temperature (blue), density (red), $^{12}\text{C}$ mass fraction (brown), $^{28}\text{Si}$ mass fraction (orange), and $\delta_{56}$ (green). The solid lines present the results with the input physics of Khokhlov (1989), the dashed lines are with the addition of the Coulomb correction terms to the NSE, and the dotted lines are the results with the default input physics. The green points mark the locations where $|\delta_{56}| = 10^{-3}$.

that the default results are reproduced by adding the missing isotopes from NSE7 with $Z \leq 14$ and from the $\alpha$-ext lists to the list used by Khokhlov (1989), which increases the number of isotopes to 161. In fact, the results from NSE4 deviate by less than 10% for this upstream density (see Figure 13), which shows that with 137 isotopes (although somewhat different from the 114 used by Khokhlov (1989)) better results can be obtained.

5.1.6 Comparison to Townsley et al. (2016)

Townsley et al. (2016) calculated the detonation wave structure for an initial composition of $X(^{12}\text{C}) = 0.5$, $X(^{16}\text{O}) = 0.48$, $X(^{22}\text{Ne}) = 0.02$ (CONe), an upstream temperature of $T_{0,9} = 0.4$ and a few values of the upstream density in the range of $[5 \times 10^6, 2 \times 10^8] \text{g/cm}^3$. The calculation were performed with TORCH (Timmes 1999), which uses the Helmholtz EOS. The list of isotopes included 200 isotopes, and screening was applied for the reaction rates. We concentrate on the overdriven detonation in which $\rho_{0,7} = 1$ and $D = 1.166 \times 10^4$ km/s, for which Townsley et al. (2016) provide detailed results. We calculate the detonation wave structure for this case by using the Helmholtz EOS, the TORCH200 isotope list (without $^{8}\text{Be}$ and $^{9}\text{B}$, see Section 3.2, which sums up to 203 isotopes), and using the option of the extended screening of MESA. As the other input physics, we use our usual default values. Since neither the extended screening nor the screening used by TORCH respect a detailed balance, the integration does not terminate at NSE, but rather at some other steady-state config-

\[ ^{28}\text{Si} \]

Townsley et al. (2016) probably used the TORCH200 net, which actually contains 205 isotopes.
uration. We integrate up to \( t = 10 \text{ s} \), at which point this steady state was obtained.

The deviation of our results (Figure 16, dashed lines) from those of Townsley et al. (2016, solid lines) is quite small. For example, the deviation in the pressures is smaller than 2%. This difference is probably because of the somewhat different reaction rates and screening factors incorporated into each of the two calculations. A calculation with our default input physics is presented as well in Figure 16 (dotted lines). As usual, the integration is performed up to \( \delta_{\text{max}} = 10^{-3} \). Larger deviations are obtained between the default calculation and the results of Townsley et al. (2016). For example, a deviation of \( \approx 7\% \) is obtained in the pressure at a distance of \( x \approx 10^3 \text{ cm} \). It is evident that the NSE values obtained with our default input physics deviate by a few percent from the steady-state configuration obtained by Townsley et al. (2016). The easiest way to analyse these differences is to compare their NSE states (which are independent of reaction rates), and as explained above, such a state does not exist for the input physics of Townsley et al. (2016).

With respect to figure 1 of Townsley et al. (2016), since there the pathological detonation speed was not calibrated to high accuracy and the sonic point location was determined by the location of the density minimum, the position of the \(^{28}\text{Si} \) abundance maximum and the sonic point location are not adequate for an accurate comparison.

### 5.2 The structure of the detonation wave in He

In this section, we present the structure of the detonation wave in He. In Section 5.2.1, we present an example of the structure of a detonation wave for some specific initial conditions. In Section 5.2.2, we calculate the structure of the detonation wave as a function of the upstream density. We then comment on the uncertainty of the results in Section 5.2.3. Finally, we compare out results to Khokhlov (1989) in Section 5.2.4.

#### 5.2.1 An example for He: \( \rho_{0,7} = 1 \) and \( T_{0,9} = 0.2 \)

We present in Figure 17, as an example, the structure of a detonation wave for He, \( \rho_{0,7} = 1 \), \( T_{0,9} = 0.2 \) and a detonation speed of \( D = 1.432 \times 10^4 \text{ km/s} \) (\( \sim D_{\text{CJ}} \approx 1.4304 \times 10^4 \text{ km/s} \) for these upstream conditions, see Table 8). The structure of this detonation wave is very different from the structure of a detonation wave in CO. The burning of \(^{4}\text{He} \) immediately synthesizes heavy elements with \( A \approx 55 \) (see detailed discussion in Khokhlov (1984) and a somewhat more accurate description in Khokhlov & Ergma (1985)). This mode of burning depletes the \(^{4}\text{He} \) by 10(50)% at \( x \approx 1.4 \times 10^3(4.0 \times 10^3) \text{ cm} \) (blue points in the lower panel), while increasing \( \tilde{Y} \) and \( \tilde{A} \), almost without changing \( \tilde{A} \), and releasing \( \approx 1.1 \text{ MeV/m}_{\text{p}} \). Most of the energy is being release with the plasma not in NSE, as \( |\delta_{56}(x) - \delta_{38}(x)| \approx 0.01 \) at \( x \approx 7.8 \times 10^3 \text{ cm} \) (orange point in the middle panel), where already \( \approx 0.77 \text{ MeV/m}_{\text{p}} \) have been released.

The middle panel shows that \( \tilde{Y} \) increases towards the NSE value (compare with Figure 6, in which \( \tilde{Y} \) decreases towards the NSE value), and we verified that the increase is controlled by the triple- \( \alpha \) reaction, \(^{3}\text{He} \rightarrow ^{12}\text{C} \). The middle panel shows that \( |\delta_{56}| \approx 0.1 \) at \( x \approx 2.4 \times 10^6 \text{ cm} \). From that position, \( |\delta_{56}| \) decreases exponentially with an \( \epsilon \)-folding distance of \( \delta_{40} \approx 2.6 \times 10^6 \text{ cm} \). The brown point marks the location where \( |\delta_{56}| = 10^{-3} \). As usual, we stop the integration when \( \delta_{\text{max}} = 10^{-3} \). The deviation of the solution parameters at the end of the integration from the NSE values (points at the right edges of the panels), which are calculated only from conservation laws, is smaller than \( 10^{-3} \). The middle panel shows that the value of \( \delta_{40} \) increases towards NSE and is \( \approx 10^{-5} \) at the end of the integration. This demonstrates the high accuracy of our integration.

#### 5.2.2 The dependence of the burning scales on the upstream density for He

For He, the detonation is of the CJ type (see detailed discussion in Section 6). Different scales of the He CJ detonation are shown in Figure 18. For low densities, \( \rho_{0,7} \lesssim 0.30 \), we are unable to inte-
grate with high accuracy up to the location where $|\delta_{56}| = 10^{-3}$, so this location and $t_{56}$ are not shown for these densities. The numerical accuracy of all scales in Figure 18 is $\lesssim 10^{-3}$.

For high upstream densities, $\rho_{0,7} \gtrsim 0.015$, the ordering of the different scales as a function of the upstream density is similar to the case of $\rho_{0,7} = 1$ that was described in detail in Section 5.2.1. The burning of $^4$He synthesizes heavy elements with $\delta \approx 55$ much faster than the rate in which $^3$He is depleted. At lower upstream densities, the depletion rate of $^4$He is faster than the rate at which heavy elements are synthesized. The energy release roughly follows the $^4$He depletion, and most of the energy is being release with the plasma not in NSQE. The reactions that dominate the approach to NSQE are shown in Figure 19 (in this case the same reactions dominate both at $|\delta_{56} - \delta_{28}| = 10^{-2}$ and at $|\delta_{56} | = 10^{-3}$). The approach to NSQE is controlled at low upstream densities, $0.3 \lesssim \rho_{0,7} \lesssim 10$, by the triple-$\alpha$ reaction, $^3\text{He} \rightarrow ^{12}\text{C}$, and to some extent by $n+p \rightarrow ^2\text{H}$, while at high densities $n + p \rightarrow ^2\text{H}$ is the dominant process with an additional contribution from $^3\text{He} \rightarrow ^1\text{H} + p$.

The scales themselves shorten significantly as the upstream density increases, due to the rise in the post-shock temperature. Furthermore, the temperature at the CJ NSQE state increases monotonically with $\rho_0$, which decreases both $\bar{A}$ and $q_{01}$ at these states (see Table 8). We mark with dashed lines in the bottom panel of Figure 18 the upstream densities in which some values of $q_{01}$ are obtained at the CJ NSQE state.

Some minor dependence of the scales on the upstream temperature are obtained (see dotted lines in Figure 20), the electron–electron term is neglected here, and it is a few percent correction for $\rho_{0,7} \lesssim 0.027$ and $T_{0,9} = 0.011$. The largest one is for the scale at which $\bar{A} = 20$ at high densities. This scale is shown as a function of the upstream temperature in Figure 21 for $\rho_{0,7} = 10$. The scale decreases as the upstream temperature increases, because the post-shock temperature, $T_s$, depends slightly on the upstream temperature. This effect is obtained at high densities, where the post-shock plasma is slightly degenerate, making the temperature a sensitive function of the pressure.

### 5.2.3 The uncertainty of the He results

The deviations of the positions where $\bar{A} = 20$, where half of the $^4$He is consumed and where $|\delta_{56}| = 10^{-3}$, calculated with the NSE4, NSE5 and NSE6 isotope lists, from the results calculated with the NSE7 isotope list are presented in Figure 22. Deviations as high as an order unity are obtained for NSE4, while the deviations of NSE5 and NSE6 are smaller than a few percent (not including $|\delta_{56}| = 10^{-3}$ near $\rho_{0,7} \approx 0.30$, where we are unable to integrate with high accuracy up to this location). The other scales shown in Figure 18 have smaller deviations. We verified that the deviations of the results obtained with the NSE7Si list deviate by less than a few percent from the results obtained with the NSE7 list. This suggests that our calculation of the length-scales is converged to a few percent. The effect of the Coulomb correction is examined in Figure 20. The Coulomb correction terms to the EOS are only important at high densities, and they change at most the $\bar{A} = 20$ scale by $\approx 15\%$. The Coulomb correction terms to the NSE have an effect at high densities, where they can decrease the length-scales by up to a factor of 2, as they increase the reaction rates. Uncertainty in the reaction rates can be at the same magnitude or even higher, making the length-scales uncertain to a factor of a few. However, a detailed study of the sensitivity to uncertain reaction rates is beyond the scope of this paper.
5.2.4 Comparing the detonation wave structure in He to Khokhlov (1989)

Khokhlov (1989) calculated the CJ detonation wave structure for He, an upstream temperature of (probably) $T_{0,9} = 0.2$ and a few values of the upstream density in the range of $\rho_0 \approx 10^4 \text{ g/cm}^3$. The value of $D_{CJ}$ used by Khokhlov (1989) is probably different from our value of $D_{CJ} = 1.4906 \times 10^4 \text{ km/s}$, calculated with the input physics of Khokhlov (1989), due to the apparent numerical bug in the EOS used by Khokhlov (1989). We compare in Figure 23 the structure of the CJ detonation. It is apparent from the upper panel of Figure 23 that the NSE state is different in the two calculations. This difference is similar in magnitude to the one we found in Section 4.2.2, suggesting that it is due to the shortcomings of the EOS used by Khokhlov (1989). Note, however, that in Table 11 we consistently get for CJ detonations a higher $T_{CJ}$ and lower $\phi_{0,1,CJ}$ than the results of Khokhlov (1988), which is not the case for the NSE state in Figure 23. This could suggest that the results of Khokhlov (1988) are inconsistent with the results of Khokhlov (1989). The abundance of the isotopes shown in the bottom panel of Figure 23 are similar in the two calculations.

We next compare in Figure 24 our results with the input physics of Khokhlov (1989, solid lines) to the results with our default input physics (dotted lines). The synthesis of heavy elements is significantly faster in the default case (compare the profile of $\breve{A}$). The inclusion of the Coulomb correction term for the NSE (dashed
Figure 21. The scale at which $\tilde{A} = 20$ (blue) and the post-shock temperature (red) as a function of the upstream temperature for He and $\rho_{0,7} = 10$.

Figure 22. The deviations of the positions where $\tilde{A} = 20$ (black), where half of the $^4$He is consumed (blue) and where $|\delta_{56}| = 10^{-3}$ (green), calculated with the NSE4 (dotted lines), NSE5 (dashed lines) and NSE6 (solid lines) isotope lists, from the results calculated with the NSE7 isotope list, for He with $T_{0,9} = 0.2$, as a function of the upstream density.

Figure 23. Figures 10 and 11 of Khokhlov (1989). The structure of a CJ detonation wave for He, $T_{0,9} = 0.2$, $\rho_{0,7} = 0.5$ and $D = 1.233 \times 10^4$ km/s, as a function of the distance behind the shock. Black lines are the results of Khokhlov (1989), while the coloured lines are our results with the input physics of Khokhlov (1989). The value of $D_{CJ}$ used by Khokhlov (1989) is probably different from our value of $D_{CJ} = 1.4906 \times 10^4$ km/s due to the apparent numerical bug in the EOS used by Khokhlov (1989). The green dashed line in the bottom panel is $\tilde{A}$.

6 AN APPROXIMATE CONDITION FOR CJ DETONATIONS

In Section 5.1.2, we found that CO detonations are pathological for all upstream densities values, as far as our numerical accuracy allowed us to test this. In Section 5.2.2, we claimed, without justifying it, that He detonations are of the CJ type. In this section, we show that He detonations are indeed of the CJ type, and we further provide an approximate condition, independent of reaction rates, that allows to estimate whether arbitrary upstream values (including composition) will support a detonation of the CJ type.

For each upstream value, we can calculate the $\tilde{Y}_0$ of the initial conditions and the $T_{CJ}$ of the NSE state for a CJ detonation. The assumption we make now is that along the detonation wave, $\tilde{Y}$ is...
monotonic between $\tilde{Y}_0$ and $\tilde{Y}_{\text{CJ}}$. This behaviour holds for CO and He (see e.g. Figures 6 and 17), but certainly breaks down when $\tilde{Y}_0 \approx \tilde{Y}_{\text{CJ}}$. Our analysis is, therefore, approximate in the sense that it applies only when $\tilde{Y}_0$ and $\tilde{Y}_{\text{CJ}}$ are significantly different. Under our assumption, there are two cases – either $\tilde{Y}$ is monotonically decreasing (as in CO detonations) or it is monotonically increasing (as in He detonations). We can, therefore, inspect the solution of the CJ detonation wave near the NSE state by solving for NSQE with $\tilde{Y}$ slightly larger or smaller than $\tilde{Y}_{\text{CJ}}$. It should be realized that for NSQE, the value of $\tilde{Y}$ completely defines the state of the plasma for a given $D_{\text{CJ}}$. This allows us to calculate $\delta \tilde{Y} = q(\tilde{Y}_{\text{CJ}}) - q(\tilde{Y}_{\text{CJ}} + \delta \tilde{Y})$ near the NSE state (with $\delta \tilde{Y} > 0$ for decreasing $\tilde{Y}$ and with $\delta \tilde{Y} < 0$ for increasing $\tilde{Y}$). In the case that $\delta \tilde{Y} > 0$ ($\delta \tilde{Y} < 0$, the energy release increases (decreases) towards the NSE state, which is the signature of a CJ (pathological) detonation. For all the cases that we examined, we find that

$$\left(\frac{dq}{d\tilde{Y}}\right)_{D_{\text{CJ}},\text{NSE}} > 0, \quad \text{(20)}$$

but we are unable to provide a proof for it. If Equation (20) always holds, then we get the following simple condition for a CJ detonation:

$$\tilde{Y}_0 < \tilde{Y}_{\text{CJ}}. \quad \text{(21)}$$

To test the approximate condition (21), we calculate $D_{\text{CJ}}$ and $D_*$ for $\rho_{0,7} = 10$, $T_{0,9} = 0.2$ and for a $^4\text{He}$, $^1\text{C}$, and $^1\text{H}$ mixture with $X(12\text{C}) = X(16\text{O})$ (and varying amounts of $X(4\text{He})$). The results are presented in Figure 25. For $X(4\text{He}) \lesssim 0.81$, we are able to resolve $D_* > D_{\text{CJ}}$. However, the deviation between $D_*$ and $D_{\text{CJ}}$ decreases abruptly with higher mass fractions of $^4\text{He}$, which our numerical accuracy does not allow us to resolve. The abrupt decrease suggests that for $X(4\text{He}) \gtrsim 0.81$ the detonation is of the CJ type, which supports the claim that He detonations are of the CJ type. Furthermore, the approximate condition (21) predicts the transition to happen at $X(4\text{He}) \approx 0.85$, which is in agreement with the detailed calculations.

7 THE EFFECT OF WEAK REACTION ON THE RESULTS

In this section, we justify the assumption of the absence of weak reactions throughout the paper. Physically, since neutrinos are lost from the system, energy constantly leaves the system and a steady-state solution cannot be obtained. However, this effect can be smaller than the numerical accuracy of the integration, allowing, for example, the condition $\delta_{\text{max}} = 10^{-3}$ to be fulfilled. We test the effects of weak reactions separately for thermal neutrino emission (NEU module of MESA) and for weak nuclear reactions (WEAKLIB module of MESA). We calculate overdriven detonations for the cases in Tables 2 with $D = D_* + 10\text{ km/s}$ (and for the cases in Table 8 with $D = D_{\text{CJ}} + 10\text{ km/s}$) with and without weak reactions. For CO, the deviation in the carbon-burning length-scale is completely negligible. The deviation in the position of the $^{28}\text{Si}$ maximum is not negligible only for $\rho_0 = 10^6 \text{ g/cm}^3$ (where there is enough time for the neutrino losses to be significant); however, in this case the maximum position is much larger than the dynamical scale. For He, the deviation in the positions where $\tilde{A} = 20$ and where half of the $^4\text{He}$ is consumed is negligible. We further compare the position in which the density profile deviates by more than 1% from the default case. It is either that the condition $\delta_{\text{max}} = 10^{-3}$ is fulfilled and there is no deviation larger than 1%, or that the deviation happens at scales comparable to (or much larger than) the dynamical scale. We, therefore, conclude that the assumption of absence of weak reactions is justified.
8 SUMMARY

In this work, we revisited the problem of thermonuclear detonation waves. We constructed lists of isotopes that allow the calculation of a thermonuclear detonation wave (Section 3.2) with some prescribed accuracy. For all isotopes, we used the most updated (measured) values of their mass and ground-state spin, and we provide fit parameters to the nuclear partition functions for all isotopes (Section 3.1). We examined in detail the EOS and constructed an EOS with an uncertainty in the range of one percent (Section 3.3). For this level of uncertainty, the nuclear level excitations (Section 3.3.1) and the ion–ion interaction terms (Section 3.4) must be included. It seems possible to construct an EOS with a ∼0.1% level of uncertainty (Potekhin & Chabrier 2010), but this accuracy is not required for current applications of supernovae. The EOS we constructed allows us to calculate CJ detonations with a degree of uncertainty in the percent level. We further provide the parameters of CJ detonations for initial compositions of CO (Section 4.1) and He (Section 4.2) over a wide range of upstream plasma conditions that are relevant for supernovae. By comparing to previous works, we demonstrate that this is the first time that such a level of accuracy is obtained for the calculation of CJ detonations. Our results have a numerical accuracy of ∼0.1%, which allows an efficient benchmarking for future studies. We provide all the relevant information needed to fully reproduce our results.

Our calculation of the structure of a detonation wave for both CO (Section 5.1) and He (Section 5.2) over a wide range of upstream plasma conditions, demonstrates that we are able to perform such a calculation to a numerical accuracy of ∼0.1%. Our determination of the pathological detonation speed for CO, as well as the NSE state for these detonations, is with a degree of uncertainty in the percent level. By comparing to previous works, we demonstrate that this is the first time that such a degree of accuracy has been reached. The uncertainty of different physical scales within the detonation waves is uncertain to a factor of a few, because the uncertainty is dominated by uncertain reaction rates. A detailed study of this uncertainty is beyond the scope of this work. The calculation of the physical scales is done with a numerical accuracy that is in the percent level, except for the location of the sonic point for pathological detonations, which is calculated with a numerical accuracy of a few tens of percent.

Besides providing accurate results and highlighting a few shortcomings of previous works, we report here a few new insights into the structure of thermonuclear detonation waves. We show that CO detonations are pathological for all upstream density values, as far as our numerical accuracy allowed us to test this (Section 5.1.2). This is different from previous studies, which concluded that for low upstream densities CO detonations are of the CJ type. These claims were probably due to low numerical accuracy. We further provide an approximate condition, independent of reaction rates, that allows to estimate whether arbitrary upstream values (including composition) will support a detonation of the CJ type (Section 6). Using this argument, we were able to show that CO detonations are pathological for all upstream densities and to verify that He detonations are of the CJ type, as was previously claimed for He. We also show that for CO detonations the location of the sonic point changes position in a discontinuous manner from \( x \sim 100 \text{ cm} \) to \( x \sim 10^2 \text{ cm} \) around \( n_\text{He} \approx 2.7 \).

Our analysis of the reactions that control the approach to NSE, which determines the length-scale of this stage, revealed that at high densities, the reaction \( ^{11}\text{B} + p \leftrightarrow ^{3}\text{He} \) plays a significant role, which was previously unknown. This will help to focus the effort of improving reaction-rate measurements.

The implications of the various improvements introduced in this work to supernova modelling will be studied in the future.

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APPENDIX A: DIFFERENCES BETWEEN WINVNV_V2.0.DAT AND ENSDF

For some isotopes, the values of the nuclear masses, $m_i$, included in WINVNV_V2.0.DAT differ from the most updated values given in the ENSDF data base, $m_i$. The list of isotopes for which $m_i$ differ is given in Table A1, together with their mass (excess) values. For some isotopes, the values of $J_{i,0}$ included in WINVNV_V2.0.DAT differ from the most updated values given in the ENSDF data base, $J_{i,0}$. The list of isotopes for which $J_{i,0}$ and $\tilde{J}_{i,0}$ differ is given in Table A2, together with their spin values.

APPENDIX B: THE INCONSISTENCY OF THE HELMHOLTZ EOS

Integrating Equations (4) in a highly accurate manner requires a high degree of accuracy for the partial derivatives of the pressure and the internal energy with respect to the independent variables. We have found that the Helmholtz EOS does not provide consistent values for $\partial \rho / \partial \rho$ at high temperatures and low densities. In order to demonstrate this inconsistency, we use the version of Helmholtz EOS with the densest grid (20 entries per decade; 'four times nominal grid' of Timmes & Swesty (2000))\textsuperscript{27}, available through Frank Timmes website\textsuperscript{28}. We consider the parameters $\rho_7 = 0.01$, $T_9 = 10$ and $Y_e = 0.5$, and we compare the electron–positron pressure, $p_{ep}$, and the derivative of this pressure with respect to the density, $\partial p_{ep} / \partial \rho$, as calculated by the Timmes EOS (red) and by the Helmholtz EOS (blue). The lower panel is a zoomed version of the upper panel, and includes linear approximations to the EOSs (black), taken with a finite differencing.

Figure B1. The electron–positron pressure, $p_{ep}$, as a function of density ($\rho_9 = \rho g (\text{cm})^{-1} = 1$) for $T_9 = 10$ and $Y_e = 0.5$, as calculated by the Timmes EOS (red) and by the Helmholtz EOS (blue). The lower panel is a zoomed version of the upper panel, and includes linear approximations to the EOSs (black), taken with a finite differencing.

\textsuperscript{27} Note that the tables provided by MESA and FLASH are with 10 entries per decade.

\textsuperscript{28} http://cococubed.asu.edu/
APPENDIX C: CORRECTIONS TO THE EXPONENTIAL MASS FORMULA OF CAMERON & ELKIN (1965)

It seems that the exponential mass formula of Cameron & Elkin (1965) contains possible errors and that the following corrections are required:

(i) The pre-factors for $E_c$ and $E_{ex}$ (p. 1291) should be $Z^2/A^{1/3}$ and $Z^{1/3}/A^{1/3}$ and not $Z^2/\alpha A^{1/3}$ and $Z^{1/3}/\alpha A^{1/3}$, respectively.

(ii) The fourth term inside the parentheses in the $E_{ex}$ expression should include the factor $r_0^3$ and not $r_0$.

(iii) The value for $\beta$ (p. 1292) should be $-35.939$ (given for $\gamma$ by Cameron & Elkin (1965)).
Table A2. The list of isotopes for which the values of $J_{i,0}$ included in winvn_v2.0.dat differ from the most updated values given in the ENSDF database, $J_{i,0}$.

| Isotope | $J_{i,0}$ | $J_{i,0}$ | Isotope | $J_{i,0}$ |
|---------|----------|----------|---------|----------|
| Be      | 1/2      | 1/2      | N        | 2        |
| O       | 1/2      | 5/2      | O        | 3/2      |
| F       | 0/2      | 5/2      | Ne       | 3/2      |
| Ne      | 1/2      | 3/2      | Na       | 3/2      |
| Mg      | 3/2      | 5/2      | Mg       | 3/2      |
| Al      | 3/2      | 5/2      | Al       | 3/2      |
| Si      | 5/2      | 7/2      | Si       | 3/2      |
| P       | 2/4      | 0        | P        | 0        |
| S       | 3/2      | 7/2      | S        | 3/2      |
| Cl      | 2/4      | 0        | Cl       | 0        |
| Ar      | 1/2      | 5/2      | Ar       | 3/2      |
| K       | 1/2      | 3/2      | Ca       | 3/2      |
| Sc      | 1/2      | 3/2      | Sc       | 3/2      |
| Ti      | 3/2      | 5/2      | Ti       | 3/2      |
| V       | 2/1      | 0        | V        | 0        |
| Cr      | 2/1      | 0        | Cr       | 0        |
| Mn      | 3/2      | 1/2      | Mn       | 3/2      |
| Mn      | 3/2      | 5/2      | Mn       | 3/2      |
| Co      | 4/6      | 0        | Co       | 0        |
| Ni      | 1/2      | 9/2      | Ni       | 1/2      |
| Cu      | 3/4      | 0        | Cu       | 0        |
| Cu      | 1/2      | 0        | Cu       | 0        |
| Ge      | 1/2      | 3/2      | Ge       | 3/2      |
| As      | 0/4      | 0        | As       | 0        |
| Se      | 3/2      | 1/2      | Se       | 3/2      |
| Br      | 9/2      | 5/2      | Br       | 5/2      |
| Br      | 3/1      | 0        | Br       | 0        |
| Kr      | 9/2      | 5/2      | Kr       | 3/2      |

(iv) The value for $\gamma$ should be $-26.587$ (given for $-\beta$ by Cameron & Elkin (1965)).

(v) The mass excess is actually given in the $^{16}$O scale (and not in the $^{12}$C scale, as claimed by Cameron & Elkin (1965)).

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