We present a high-resolution convergence study of detonation initiated by a temperature gradient in a stoichiometric hydrogen–oxygen mixture using the Pencil Code. With Mach numbers reaching 10–30, a certain amount of shock viscosity is needed to remove or reduce numerical pressure oscillations on the grid scale at the position of the shock. Detonation is found to occur for intermediate values of the shock viscosity parameter. At fixed values of this parameter, the numerical error associated with those small wiggles in the pressure profile is found to decrease with decreasing mesh width $\delta x$ like $\delta x^{-1.4}$.

**Keywords:** Combustion; numerical methods; detonation; shock waves; chemical reaction.

## 1. Introduction

Detonation can be produced by the coupling of a spontaneous reaction wave, which propagates along an initial temperature gradient, with a pressure wave (Zeldovich et al. 1970, Zeldovich 1980). This process is governed by the time-dependent compressible reactive Navier-Stokes equations. Its direct numerical simulation (DNS) is an intricate problem that is of fundamental importance for understanding the ignition of different combustion modes caused by a transient thermal energy deposition localised in a finite volume of reactive gas (Liberman et al. 2012). High resolution methods are necessary to resolve the broad range of length scales. It is also well-known that problems involving strong shocks, such as in the final stage of the deflagration to detonation transition (DDT), require the use of shock-capturing techniques to eliminate or reduce spurious oscillations near discontinuities. One of the widely used approaches is the use of weighted essentially non-oscillating (WENO) finite differences (Jiang and Shu 1996), which is an improvement upon the essentially non-oscillating (ENO) scheme. The main idea of the WENO scheme is to use a convex combination of all the candidate stencils rather than the smoothest candidate stencil to achieve a higher order accuracy than the ENO scheme, while maintaining the essentially non-oscillating property near discontinuities. There are also other methods such as the Total Variation Diminishing (TVD) method or the Artificial Compression...
Method (ACM) switch (Lo et al. 2007).

Yet another approach to avoid wiggles in the numerical solution is to add a shock-capturing viscosity. However, one must be cautious when using such a shock-capturing viscosity, since its properties are problem-dependent. The shock-capturing viscosity will fail to eliminate oscillations if it is too small. Since the gaseous combustion process is highly sensitive to the resolution of the reaction zone, using too large shock-capturing viscosity can lead to an artificial coupling of the leading pressure wave and the flame front. Thus, it is essential to determine the proper shock-capturing viscosity when using the PENCIL CODE to simulate problems involving the onset of detonation.

The test problem examined in this paper is the hot spot problem, which is a chemically exothermic reactive mixture with a nonuniform distribution of temperature. According to the theory developed by Zeldovich et al. (1970) and Zeldovich (1980), the gradient of induction time associated with temperature (or concentration) gradients may be ultimately responsible for the detonation initiation. A similar concept of shock-wave amplification by coherent energy release (SWACER) was introduced later by Lee and Moen (1980). The basic idea is that a spontaneous reaction wave can propagate through a reactive gas mixture if there is a spatial gradient in the chemical induction time $\tau_{\text{ind}}$. The spontaneous reaction wave is ignited first at the location of minimum induction (ignition delay) time $\tau_{\text{ind}}$ and then spreads by spontaneous ignition over neighbouring locations where the temperature is lower and $\tau_{\text{ind}}$ is correspondingly longer. The velocity of the spontaneous reaction wave is analogous to a phase velocity. It cannot be smaller than the velocity of deflagration, but is not limited from above, and depends on the steepness of the temperature gradient and the temperature derivative of the induction time. The proposed mechanism of detonation initiated by the temperature gradient suggests that the formation of an induction time gradient produces a spatial time sequence of energy release, which then produces a compression wave that gradually amplifies into a shock wave. Coupling of the spontaneous reaction and pressure waves can cause shock wave amplification by coherent energy release and can finally result in the formation of a detonation wave. This requires a certain synchrony between the progress of the shock and the sequential release of chemical energy by successive reactions along the temperature gradient.

The first demonstration of the ignition of a detonation wave by a temperature gradient was by Zeldovich et al. (1970). Although this earliest numerical simulations had a low resolution, the authors demonstrated successfully that sufficiently shallow gradients produce detonation, while for steeper gradients the reaction wave and the shock failed to couple together. In subsequent studies, Zeldovich et al. (1988), He and Clavin (1992), He (1996), Khokhlov et al. (1997), Bartenev and Gelfand (2000), and Kurtz and Regele (2014) have employed a one-step chemical model to investigate regimes of detonation ignition by an initial temperature gradient. However, the one-step model or other simplified chemical models do not predict correctly the induction time for the combustion process involving a large set of chain-branching reactions. Liberman et al. (2011, 2012) studied different modes of combustion produced by the initial temperature gradient in stoichiometric hydrogen–oxygen and hydrogen–air mixtures ignited by a temperature gradient using detailed chemical models and compared the results with those obtained with a one-step chemical model. In particular, it was shown that the minimal slope of the temperature gradient required for triggering detonation and other combustion modes obtained in simulations with simplified chemical models, for example a one-step model, is orders of magnitude smaller than those obtained in simulations with a detailed chemical model. Wang et al. (2018) and Liberman et al. (2018) studied the influence of the chemical reaction model on detonation ignited by a temperature gradient for hydrogen-air and methane-air mixtures. They concluded that the one-step model and other simplified models usually cannot describe correctly the ignition processes. Thus, using simplified chemical kinetics for understanding the mechanisms of DDT must be considered with great caution.

The aim of this paper is to study the convergence of detonations simulation using the
PENCIL CODE. The paper is organised as follows. In section 2, the governing equations are presented and the setup of the hot spot problem is described. Section 3 presents a convergence study of the pressure profiles obtained using the PENCIL CODE. The dependence on the shock viscosity is also investigated in this section. In section 4 we conclude by summarising our main findings.

2. The model

2.1. The basic equations

The set of equations for modelling combustion was implemented into the PENCIL CODE by Babkovskai et al. (2011). Considering a mixture of \( N_s \) species undergoing \( N_r \) reactions, we solve the continuity equation for the total density \( \rho \),

\[
\frac{D\ln \rho}{Dt} = -\nabla \cdot U, \tag{1}
\]

the momentum equation for the velocity \( U \),

\[
\frac{D U}{Dt} = -\frac{1}{\rho} \nabla p + 2\frac{\rho}{\rho} \nabla \cdot \tau, \tag{2}
\]

the energy equation for the temperature \( T \),

\[
c_v \frac{D \ln T}{Dt} = \sum_{k=1}^{N_s} \frac{DY_k}{Dt} \left( \frac{R}{W_k} \frac{h_k}{T} \right) - \frac{R}{W} \nabla \cdot U + \frac{\tau \cdot \nabla U}{\rho T} - \frac{\nabla \cdot q}{\rho T}, \tag{3}
\]

and the equation for the mass fraction of the \( k \)th species \( Y_k \) in the form

\[
\rho \frac{DY_k}{Dt} = -\nabla \cdot J_k + \dot{\omega}_k, \tag{4}
\]

where \( D/Dt = \partial/\partial t + U \cdot \nabla \) is the advective derivative and \( \tau_{ij} = 2\rho \Sigma_{ij} + \rho \zeta \delta_{ij} \nabla \cdot U \) are the components of the stress tensor with \( \Sigma_{ij} = \frac{1}{2}(\partial U_i/\partial x_j + \partial U_j/\partial x_i) - \frac{1}{3} \delta_{ij} \nabla \cdot U \) being the components of the traceless rate-of-strain tensor, \( \nu \) is the kinematic viscosity, \( \zeta \) is the bulk viscosity, \( \dot{\omega} \) is the reaction rate and subscript \( k \) refers to species number \( k \). The pressure is given by the equation of state,

\[
p = \rho T \frac{R}{W} = \rho T \sum_{k=1}^{N_s} \left( \frac{Y_k}{W_k} \right), \tag{5}
\]

where \( R, W, \) and \( W_k \) are the universal gas constant, the molecular weight of species \( k \), and the mean molecular weight of the mixture, respectively. The viscosity of species \( k \) is given by Coffee and Heimerl (1981) as

\[
\mu_k = \frac{5}{16} \frac{\sqrt{\pi k_B T m_k}}{\sigma_k^2 \Omega_k^{(2,2)*}}, \tag{6}
\]

where \( \sigma_k \) is the Lennard-Jones collision diameter, \( k_B \) is the Boltzmann constant, \( m_k \) is the mass of the molecule, and \( \Omega_k^{(2,2)*} \) is the collision integral (see Mourits and Rummens 1977). Then, the viscosity of the mixture, \( \mu = \rho \nu_{mix} \), is given by Wilke (1950)

\[
\mu = \sum_{k=1}^{N_s} \left( X_k \mu_k / \sum_{j=1}^{N_s} X_j \Phi_{kj} \right). \tag{7}
\]
Here, $X_k$ is the mole fraction of species $k$ and $\Phi_{kj}$ is given by

$$\Phi_{kj} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_k}{W_j}\right)^{-1/2} \left[1 + \left(\frac{\mu_k}{\mu_j}\right)^{1/2} \left(\frac{W_j}{W_k}\right)^{1/4}\right]^2.$$  (8)

The heat flux $q$ is given by

$$q = \sum_{k=1}^{N_s} h_k J_k - \lambda \nabla T.$$  (9)

Here, $J_k = \rho Y_k V_k$ is the diffusive flux. Fick’s law is employed to calculate the diffusion velocity $V_k$ as [Poirinsot and Veynante 2005]

$$V_k = -\frac{D_k}{X_k} \nabla X_k,$$  (10)

where the diffusion coefficient for species $k$ is expressed as

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k} X_j / D_{jk}},$$  (11)

and the binary diffusion coefficient is given by

$$D_{jk} = \frac{3 \sqrt{\pi k_B^3 T^3/m_{jk}}}{16 \pi \sigma_{jk}^2 \Omega_{jk}^{(1,1)*}},$$  (12)

where $\Omega_{jk}^{(1,1)*}$, $\sigma_{jk}$, and $m_{jk}$ are given by Evlampiev (2007).

The thermal conductivity for pure species $k$ is expressed as

$$\lambda_k = \frac{\mu_k}{W_k} \left(f_{\text{trans}} \cdot C_{v,\text{trans}} + f_{\text{rot}} \cdot C_{v,\text{rot}} + f_{\text{vib}} \cdot C_{v,\text{vib}}\right),$$  (13)

and the thermal conductivity of the mixture follows an empirical law. The specific heat $c_{p,k}$ and specific enthalpy $h_k$ of species $k$ are calculated by using tabulated polynomials used in rocket science by the National Aeronautics and Space Administration (NASA) and are known as NASA polynomials. We use here the coefficients from Kéromnès et al. (2013).

The expression for the reaction rate is [Poirinsot and Veynante 2005]

$$\dot{\omega}_k = W_k \sum_{s=1}^{N_r} \left(\nu_{ks}^{\prime\prime} - \nu_{ks}^{\prime}\right) \left[ k_{t,s} \prod_{j=1}^{N_r} \left(\rho_j / W_j\right)^{\nu_{js}^{\prime}} - k_{r,s} \prod_{j=1}^{N_r} \left(\rho_j / W_j\right)^{\nu_{js}^{\prime\prime}}\right],$$  (14)

where $\rho_k$ is the density of species $k$. Furthermore, $\nu_{ks}^{\prime}$ and $\nu_{ks}^{\prime\prime}$ are the stoichiometric coefficients of species $k$ of reaction $s$ on the reactant and product sides, respectively. Furthermore, $k_{t,s}$ is the forward rate of reaction $s$, which is given by

$$k_{t,s} = B_s \alpha_s \exp(-E_s / RT),$$  (15)

where $B_s$ is a pre-exponential factor, $\alpha_s$ is the temperature exponent, and $E_s$ is the activation energy. These are all empirical coefficients that are given by the kinetic mechanism. The backward rate of reaction $s$ is calculated from the forward rates through the equilibrium constant

$$k_{r,s} = k_{t,s} / k_{c,s},$$  (16)

where $k_{c,s} = (p_0 / RT)^{\sum_{s=1}^{N_r} (\nu_{ks}^{\prime\prime} - \nu_{ks}^{\prime}) \exp(\Delta S_s / R - \Delta H_s / RT)}$. Here $p_0 = 1$ bar, $\Delta S_s$ and $\Delta H_s$ are entropy and enthalpy changes for reaction $s$. The detailed chemical mechanism chosen to simulate the hot spot problem is the mechanism developed by Kéromnès et al. (2013).
which includes \( N_r = 19 \) reactions and \( N_s = 8 \) species. The induction time of this mechanism, which is one of the important parameters for the simulation, has been validated by extensive experiments and simulations at pressure from 1 to 70 bar, over a temperature range of 914 K to 2200 K.

The shock viscosity of von Neumann and Richtmyer (1950) is applied as a bulk viscosity,

\[
\zeta = C_{\text{shock}} \delta x^2 \langle -\nabla \cdot U \rangle_+,
\]

and is required to eliminate wiggles in the numerical solution. Here, \( \langle \ldots \rangle_+ \) denotes a running five point average over all positive arguments, corresponding to a compression.

### 2.2. Setup of the problem

We consider an unburned gas mixture under uniform initial conditions except for the aforementioned linear temperature gradient. The initial conditions at \( t = 0 \) are constant pressure and zero velocity of the unburned mixture. On the left boundary at \( x = 0 \), we assume a reflecting wall, where \( U_x(x=0,t) = 0 \) and the initial temperature, \( T(x=0) = T^* \) exceeds the ignition threshold value. Thus, the initial conditions are as follows:

\[
\begin{align*}
T(x,0) &= \begin{cases} 
T^* - (T^* - T_0) x/L, & 0 \leq x \leq L, \\
T_0 & x > L,
\end{cases} \\
p(x,0) &= p_0, \\
U(x,0) &= 0.
\end{align*}
\]

According to the Zeldovich gradient mechanism, the reactions begin at the temperature maximum, \( T^* \), and then propagate along the temperature gradient due to spontaneous auto-ignition of the mixture. The velocity of the spontaneous reaction wave,

\[
U_{\text{sp}} = \frac{dx}{d\tau_{\text{ind}}} = \left( \frac{d\tau_{\text{ind}}}{dT} \right)^{-1} \left( \frac{dT}{dx} \right)^{-1}
\]

depends on \( d\tau_{\text{ind}}/dT \) and the steepness of the temperature gradient. It could be larger than that of the pressure wave, if the temperature gradient is sufficiently shallow. Then, the coupling between the spontaneous reaction wave with the shock wave, along with the coherent energy release in the reaction, cause shock wave amplification and the transition into a detonation wave. Since we only consider the process of detonation initiation, the parameters in equation (18) are chosen as follows:

\[
T^* = 1500 \text{ K}, \quad T_0 = 300 \text{ K}, \quad L = 8 \text{ cm}, \quad p_0 = 1 \text{ bar}.
\]

This set of parameters was also used by Liberman et al. (2012) to produce a steady detonation wave in a stoichiometric hydrogen–oxygen mixture.

### 3. Results

#### 3.1. General remarks regarding the transition to detonation (TD)

In the absence of shock viscosity, or when the shock viscosity is too small, small-scale oscillations on the grid scale (wiggles) occur. Such a solution cannot be numerically reliable and must be discarded. When we add shock viscosity, the wiggles become weaker. However, when the shock viscosity is too large, TD is no longer possible. Thus, to pose a meaningful convergence test, we decided to fix the value of \( C_{\text{shock}} \) to a relatively small value of 0.8 and then increase the resolution. This means that the shock viscosity continuously decreases with increasing resolution until it becomes negligible.
Table 1. Summary of the fit parameters at $t = 42 \mu s$; $x_0$ is in cm, $p_0$ and $p_1$ are in bar, $p'_1$ is in $\text{bar} \mu \text{m}^{-1}$, $L_1$ and $L_2$ are in $\mu \text{m}$, and $\delta t_{\text{min}}$ in ps. Runs (a)–(d) have $C_{\text{shock}} = 0.8$ and run (e) has $C_{\text{shock}} = 0.2$.

<table>
<thead>
<tr>
<th>$\delta x$</th>
<th>$x_0$</th>
<th>$p_1$</th>
<th>$p'_1$</th>
<th>$L_1$</th>
<th>$L_2$</th>
<th>$N_x$</th>
<th>$N_t$</th>
<th>$\delta t_{\text{min}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) 1.993</td>
<td>9.37498</td>
<td>35.00</td>
<td>0.2200</td>
<td>2.56</td>
<td>0.36</td>
<td>50,176</td>
<td>392,000</td>
<td>42</td>
</tr>
<tr>
<td>(b) 0.997</td>
<td>9.4825</td>
<td>31.20</td>
<td>0.0546</td>
<td>1.21</td>
<td>0.30</td>
<td>100,352</td>
<td>1,266,600</td>
<td>24</td>
</tr>
<tr>
<td>(c) 0.498</td>
<td>9.44390</td>
<td>33.21</td>
<td>0.0535</td>
<td>0.442</td>
<td>0.0587</td>
<td>200,704</td>
<td>2,826,300</td>
<td>12</td>
</tr>
<tr>
<td>(d) 0.199</td>
<td>9.27530</td>
<td>35.78</td>
<td>0.1128</td>
<td>0.1145</td>
<td>0.0157</td>
<td>501,760</td>
<td>14,603,000</td>
<td>2.5</td>
</tr>
<tr>
<td>(e) 0.199</td>
<td>9.46444</td>
<td>28.70</td>
<td>0.0300</td>
<td>0.4069</td>
<td>0.1719</td>
<td>501,760</td>
<td>14,255,800</td>
<td>2.5</td>
</tr>
</tbody>
</table>

3.2. The pressure wave at increasing resolution

With each doubling of the number of mesh points, the total shock viscosity integrated over the width of the shock decreases by a factor of four. In addition, there is the time-dependent molecular viscosity profile which is independent of the mesh resolution. Thus, we expect that in the limit of infinite resolution, which yields a vanishing shock viscosity, the wiggles of the tip of the pressure profile should disappear. To test this assertion, and to study the corresponding convergence property of the code, we perform four simulations with mesh resolutions between $\delta x = 2 \mu \text{m}$ and $0.2 \mu \text{m}$ using $C_{\text{shock}} = 0.8$; see table I. The corresponding pressure profiles are shown in figure [I] for the four cases (a)–(d). The insets in each panel show the corresponding pressure profile in the proximity of the peak.

![Figure 1](image.png)

It is evident that the wiggles decrease as we increase the resolution. In addition, the pressure profiles change slightly with resolution. To characterise these changes, we determine a fit to the pressure peak of the form

$$p_{\text{fit}}(x, t_*) = p_0 + \left[p_1 + \left(x - x_0\right) p'_1\right] \Theta(x_0 - x),$$

where $\Theta(x)$ is the Heaviside step function (= 1 for $x > 0$ and zero otherwise), $x_0$ is the position of the peak at the last time $t_*$, $p_0$ is the atmospheric background pressure ahead of the peak, $p_1$ is the pressure increase relative to $p_0$ just behind the peak, and $p'_1$ is the slope of the pressure profile to the left of the peak, i.e., in the wake of the detonation wave. In all cases, the pressure ahead of the peak is $p_0 = 1.013 \times 10^6 \text{dyn cm}^{-2}$, which does not need to be fitted. The remaining three parameters are given in table I where the pressure is given in bar ($1 \text{ bar} = 10^6 \text{ dyn cm}^{-2}$).

Note that between the runs with $\delta x = 1 \mu \text{m}$ and $0.5 \mu \text{m}$, the front speeds (or front positions $x_0$) agree within 0.05%, but for the run with $\delta x = 0.2 \mu \text{m}$, the front speed has decreased by nearly 2%. The reason for this apparent loss of accuracy is not fully identified, although it is clear that smaller values of $C_{\text{shock}}$ lead again to larger front speeds; see run (e) in table I. It is therefore possible that at this high resolution, the value $C_{\text{shock}} = 0.8$ is already too large and that a smaller value, for example around 0.6, could be more reasonable. We should also point out that we have used a relatively optimistic choice of the viscous time step (we chose $\delta t \nu_{\text{max}}/\delta x^2 = 0.4$ instead of the more conservative value of 0.25 that is recommended in the manual to the PENCIL CODE). However, comparisons with the smaller value did not indicate any differences in the front speed. The fact that the viscous time step enters in this highest resolution run, but not in the others, is related to the extremely small mesh size in this case. This makes the time step constraint from the relatively large molecular viscosity near $x = 0$ very severe. Note also that in this run, waves appear in the wake of the pressure field behind the peak after $t = 36 \mu s$. These also seem to be spurious and are not found when $C_{\text{shock}}$ is smaller.
Convergence properties of detonation simulations

Figure 1. Pressure profiles for (a) $\delta x = 2 \mu m$, (b) $1 \mu m$, (c) $0.5 \mu m$, and (d) $0.2 \mu m$ in regular time intervals from $t = 2 \mu s$ to $42 \mu s$. The insets show the pressure peak at the last time, indicated by filled symbols, where the red line shows the fit in the proximity of the pressure peak. Note that the $x$ range varies.

Figure 1. Pressure profiles for (a) $\delta x = 2 \mu m$, (b) $1 \mu m$, (c) $0.5 \mu m$, and (d) $0.2 \mu m$ in regular time intervals from $t = 2 \mu s$ to $42 \mu s$. The insets show the pressure peak at the last time, indicated by filled symbols, where the red line shows the fit in the proximity of the pressure peak. Note that the $x$ range varies.
Next, to characterise the convergence, we use the $L_1$ and $L_2$ norms defined here as follows:

$$L_1 = \int_{x_1}^{x_2} |p(x, t_*) - p_{\text{fit}}(x, t_*)| \, dx / (p_0 + p_1),$$

(22)

$$L_2 = \int_{x_1}^{x_2} |p(x, t_*) - p_{\text{fit}}(x, t_*)|^2 \, dx / (p_0 + p_1)^2.$$

(23)

Both have the dimension of a length. These values are also given in table 1. Figure 2 shows that $L_1$ and $L_2$ decrease with resolution like $\delta x^{1.4}$.

In figure 3 we compare the molecular viscosity profile at the last time with the corresponding shock viscosity for the three highest resolutions shown in figures 1(b)–(d). The overall profile of the molecular viscosity is the same in all three cases and varies significantly from $\sim 10 \text{ cm}^2 \text{s}^{-1}$ at $x = 0$ to $\sim 0.3 \text{ cm}^2 \text{s}^{-1}$ at and ahead of the shock. However, the peak of the shock viscosity decreases from $\sim 10 \text{ cm}^2 \text{s}^{-1}$ in figure 1(b) by about a factor of five to $\sim 1.8 \text{ cm}^2 \text{s}^{-1}$ in figure 1(d). In addition, the width of the shock viscosity profile also decreases by about a factor of five, so the integrated effect of the shock viscosity diminishes by a factor of about 25, as expected from equation (17). Note that for the highest resolution, the shock viscosity makes up a small contribution compared to the molecular viscosity ($\sim 10 \text{ cm}^2 \text{s}^{-1}$ at $x = 0$) is much larger than the maximum of the shock viscosity ($\sim 1.8 \text{ cm}^2 \text{s}^{-1}$ at $x = 9.4 \text{ cm}$, although at this point the molecular value is only $\sim 0.3 \text{ cm}^2 \text{s}^{-1}$); compare figures 3(a) and 3(d). This means that at late times, when $\nu$ has become large far in the wake of the shock, an enormous amount of time is spent because the viscous time step is then so short. This is also evident from table 1, where we see that the total number of time steps has increased by a factor of over five as the resolution was increased by only a factor of 2.5.
3.3. Dependence on $C_{\text{shock}}$

Next, we investigate the dependence of our solutions on the value of $C_{\text{shock}}$. In figure 4, we show pressure profiles for different values of $C_{\text{shock}}$ at resolutions of $\delta x = 1 \mu m$ and $0.5 \mu m$. For $C_{\text{shock}} \leq 1.4$, the pressure profiles still show wiggles at the position of the pressure maximum, but the wiggles are smaller and more localized at the higher resolution of $0.5 \mu m$. For $C_{\text{shock}} = 1.4$, however, the wiggles are nearly completely negligible at a resolution of $0.5 \mu m$, but the pressure profile has also changed in that case and has now a short flank with a negative slope just behind the shock, that is, to its left. For $C_{\text{shock}} = 1.5$, TD is only found in the case with $\delta x = 1 \mu m$, but not with $\delta x = 0.5 \mu m$.

In figure 5, we show a larger portion of the wake behind the pressure front, where we see the occurrence of another type of long-wavelength oscillation, when $C_{\text{shock}}$ is larger than 0.8. Those waves are similar for both the higher and lower resolution runs, but could also be a feature of having under-resolved the solution at earlier times that are not shown here.

3.4. Speeds of pressure and reaction fronts

Finally, we show in figure 6 the time dependence of the positions and speeds of the pressure and spontaneous reaction fronts. In practice, the speeds $U_i$ (with $i = p$ for pressure and $i = sp$ for spontaneous reaction wave) are computed by time differentiation of the position $x_i$, which is obtained from the volume where the pressure or the reactant are above a certain threshold. Specifically, we compute

$$U_p = \frac{dx_p}{dt} = -\frac{d}{dt} \int_0^{x_{\text{max}}} \max(p_{\text{crit}} - p, 0)/(p_{\text{crit}} - p_0) \, dx,$$  \hspace{1cm} (24)
where we have used $p_{\text{crit}} = 1.020 \text{ bar}$ as threshold pressure and $p_0 = 1.013 \text{ bar}$ is still the same background pressure as in equation (21). The spontaneous reaction speed is based on the amount of water produced, i.e.,

$$U_{\text{sp}} = \frac{dx_{\text{sp}}}{dt} = \frac{d}{dt} \int_0^{x_{\text{max}}} \max(1 - Y_k/Y_{k0}, 0) \, dx,$$

(25)

where $k = \text{H}_2\text{O}$ and $Y_{k0} = 0.3$ is half the value of $Y_k \approx 0.6$ after $\text{H}_2$ has reacted with $\text{O}_2$. The final values of the two speeds are $U_p = 3.06 \text{ km s}^{-1}$ and $U_{\text{sp}} = 3.01 \text{ km s}^{-1}$. These values are close to the empirically determined value of $3.0 \text{ km s}^{-1}$, which is only known to within about 1% accuracy and therefore compatible with our results.

According to equation (19), the velocity of the spontaneous reaction wave decreases in the beginning, since $U_{\text{sp}} \propto (d\tau_{\text{ind}}/dT)^{-1}$. It reaches a minimum somewhere near the crossover temperature $T_{\text{cr}} \approx 1000 \text{ K}$ (for the present mixture of $\text{H}_2$ and $\text{O}_2$) for the steepest gradient capable of initiating detonation which corresponds to the transition from the endothermal to the exothermal stage of the reaction. In our case, the gradient is rather shallower, so the minimum of the velocity is reached earlier.

After reaching the minimum velocity, the speed of the spontaneous reaction wave increases
due to energy release in the reaction. To accomplish coupling between the spontaneous reaction wave and the pressure wave, it is necessary (but not sufficient) that $U_{sp} > U_p$ after the point where $U_{sp}$ is minimum, which is the case during the interval $12 \mu s \leq t \leq 19 \mu s$. For $t > 19 \mu s$, the coupling between the reaction wave and the shock wave is developing until detonation is reached at $t \approx 38 \mu s$. Note also that $U_{sp}$ is now slightly less than $U_p$, but this is natural because the reaction happens always slightly behind the leading shock. In fact, at late times, hardly any difference between $x_p$ and $x_{sp}$ can be seen; see figure 6(a). This is compatible with the experimental value of the detonation; see Kuznetsov et al. (2005).

4. Conclusions

Using high-resolution simulations of detonation initiated by an initial temperature gradient in a hydrogen–oxygen mixture, we have shown that the transition to and properties of detonation can successfully be modelled for intermediate values of the shock viscosity parameter. The numerical error, as determined by comparing with an empirical fit to the pressure peak in the final stage of TD, is found to decrease like $\delta x^{1.4}$ with decreasing mesh size. The shock
viscosity has non-vanishing values only in the immediate proximity of the shock and reaches there still values of about four times the molecular value in our highest resolution simulation. Unfortunately, the position of the shock still depends on the value of $C_{\text{shock}}$ of around 3 km s$^{-1}$. Nevertheless, the shock speed reaches the expected value in the final stage of TD.

It remains unsatisfactory that even at the largest resolution of half a million mesh points in...
just the $x$ direction, we are still unable to avoid the use of a shock viscosity. This is because the shock is so strong and the molecular viscosity still too small by comparison. Furthermore, we have been unable to demonstrate that the use of a small amount of shock viscosity does not affect the details of the shock position or even the detailed shape of the shock profile. We can therefore not be completely sure that TD will still be recovered at even higher resolution, which has not yet been possible to simulate. A reason for the current limitation is that our code is optimised to work for three-dimensional problems. It is therefore conceivable that a significant speed-up could be achieved by optimising the code for one-dimensional problems. In that case it would also be rather straightforward to use an adaptive mesh, which could make the calculations significantly more economic.

Another possible avenue for future research is to solve the governing equations in conservative form so that mass, momentum, and energy are conserved to machine procession. A difficulty here is the presence of source terms in the equations for the mass fractions of the individual species. Comparison with the WENO scheme, which does use a conservative formalism, is already in progress. Unfortunately, the WENO scheme is computationally demanding and it is difficult to reach resolutions comparable to what has been done with the PENCIL CODE. (Its typical performance is $0.05\,\mu s$ wall clock time per step and mesh point with 2048 processors on a Cray XC40 with 2.3 GHz Intel cores.) Moreover, in our preliminary investigations, it proved difficult to recover TD at high resolution. On the other hand, of course, we know from experiments that TD does occur. Thus, assuming that our equations are physically correct, as stated, there should be no doubt that any failure to recover TD must be regarded as a numerical artifact.

Yet another approach is to isolate the essence of the problem in a simpler single reaction model. One must then also use an idealised viscosity and a simplified equation of state. Those modifications could enable us to perform simulations at much higher resolution so that it is possible to focus on the purely numerical aspect of using a shock viscosity in this problem.

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