Acoustic Timescale Detonation Initiation in 2-D and its Relationship with the 1-D Description

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1 Introduction

One dimensional numerical simulations of spatially resolved thermal power deposition on the acoustic timescale have demonstrated a mechanism to achieve Deflagration-to-Detonation Transition (DDT) [1–3]. This mechanism is characterized by heating a spatially resolved localized volume of fluid with length l and sound speed a for a duration $t_{\rm h}$ that is similar in magnitude to the acoustic timescale associated with that fluid volume $t_{\rm a} = l/a$. This approach is contrasted with other approaches [4] that model detonation initiation subsequent to an instantaneous deposition of energy at a plane or a point. These approaches are only valid in the limit that $t_{\rm h} \ll t_{\rm a}$ such the dynamics associated with the creation of the initial shock wave occur fast enough that the energy is deposited in a completely constant volume process.

This work focuses on heating the fluid on a timescale where $t_{\rm h} \sim t_{\rm a}$. In this limit it becomes necessary to resolve the spatial and temporal transients involved in the creation and relaxation of the initial blast wave. It has been shown [1–3] that in this limit the fuel is consumed in a timeframe similar to the acoustic timscale producing a nearly, but not completely, constant volume reaction where the local pressure rises with temperature. Compression waves generated by the subsequent relaxation of the ephemeral high pressure spot (explosion) transition to shocks and preheat an induction zone of fluid between the lead shock and the reacted fluid. In addition to the previous work [1–3] spontaneous ignition of the induction zone has been observed by others both experimentally [5] and numerically [6].

Most of the previous one-dimensional simulations focus on non-dimensional activation energies in the range $10 - 13.8$, while more realistic activation energies can be as high as 50 or more. Previous 1-D results [3, 7] demonstrate that initiation still occurs with increased activation energy, but that a more incremental set of localized explosions occur similar to the theory proposed in Ref. [8]. It has been unclear whether the concepts developed in the previous simulations are relevant in multiple dimensions. The current work focuses on the 2-D aspects of the acoustic timescale DDT process. Multiple different 2-D simulations of acoustic timescale DDT are performed by depositing energy for a finite duration in a circular region inside of a channel. In some cases DDT is achieved and in others it fails. Explanations are presented for the differences and how transverse waves generated from the initial thermal explosion play a role in the DDT process.

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2 Problem Statement and Methodology

The non-dimensional 2-D reactive Euler equations are used to simulate detonation initiation. The equations are written in terms of the conserved quantities ρ, ρu_j, total energy ρe_T and fuel density ρY

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1a}$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial}{\partial x_i}\rho u_i u_j = -\frac{\partial p}{\partial x_j} \tag{1b}$$

$$\frac{\partial \rho e_T}{\partial t} + \frac{\partial}{\partial x_i}(\rho e_T + P)u_i = Q + \dot{W}q \tag{1c}$$

$$\frac{\partial \rho Y}{\partial t} + \frac{\partial \rho Y u_i}{\partial x_i} = -\dot{W}. \tag{1d}$$

The equation of state and reaction rate are defined

$$p = (\gamma - 1)\left(\rho e_T - \frac{1}{2}\rho u_i u_i\right) \tag{2}$$

$$\dot{W} = B\rho Y \exp(-E/T). \tag{3}$$

The reaction rate $\dot{W}$ is modeled after a simple Arrhenius reaction rate where B is the pre-exponential factor, E is the non-dimensional activation energy $E = E'/(R'T'_o)$ and $T = p/\rho$. Two additional source terms $\dot{Q}$ and $(\dot{W}q)$ are added to the energy equation for the thermal power deposition and chemical energy release.

The variables use the non-dimensionalization defined in [2] where the thermodynamic variables (p, ρ, T) are expressed with respect to the undisturbed dimensioned initial state (p'_o, ρ'_o, T'_o) and the subscript "o" indicates the initial state and prime indicates a dimensioned quantity. The entire non-dimensionalization is premised on a characteristic length l' for power deposition in the undisturbed fluid such that the acoustic timescale $t'_a = l'/a'_o$, where $a'^2_o = \gamma R'T'_o$ and $\gamma = C'_p/C'_v$.

Each simulation begins with the reactive gas at rest in thermal equilibrium with initial condition

$$\rho_o = p_o = Y_o = 1 \quad u_{jo} = 0 \tag{4}$$

with transient thermal power deposition $\dot{Q}$

$$\dot{Q} = 4.2\Big(\tanh\Big[5\,(t - t_a)\Big] - \tanh\Big[5\,(t - t_b)\Big]\Big)g(x_{\rm k}) \tag{5}$$

The geometric term $g(x_{\rm k})$ limits the power addition to a circle of radius 2 centered at $x = 0$. The domain lies in $x \in [-3, 93]$ and $y \in [-3, 12]$ and reflecting slip walls are present on all walls except the exit $x = 93$. Each simulation uses a heat of reaction $q = 15$, specific heat ratio $\gamma = 1.4$ and activation energy $E = 13.8$. Heat is added between $t_a = 0.5$ and $t_b = 5.25$.

Two separate simulations are presented where one has a pre-exponential factor $B = 35$ and successfully initiates a detonation while the second $B = 15$ does not form a detonation wave. Based on the previous work the steps leading to detonation formation include (1) thermal power deposition, (2) an initial explosion and generation of compression waves, (3) an induction period with shock propagation through the reacted fluid, (4) a localized explosion and (5) overdriven detonation wave formation. The events that occur beyond detonation formation are out of the scope of this work. Case 1 with $B = 35$ uses a grid spacing $\Delta x = \Delta y = 0.015$ on the finest level and Case 2 with $B = 15$ uses $\Delta x = \Delta y = 0.03$. The dynamically Adaptive Wavelet-Collocation Method (AWCM) is used in combination with a hyperbolic solver to perform the simulations [9]. Since the 1-D simulations [3] show a dependence on numerical resolution a grid convergence study was performed for the 2-D simulations.

3 Results

Case 1 begins with the power deposited in a circle and a chemical explosion follows. This explosion produces a strong circular compression wave that propagates away from the source as shown in the $t = 2$ pressure contour shown in Figure 1.

The compression wave reflects off the three adiabatic walls producing a geometrically complex post-reflection shock wave. The reflected wave originating from the bottom left corner is incident upon the edge of the reacted deposition region and induces a Richtmyer-Meshkov instability seen in the temperature contours for $t = 5$ and 7, which deforms the reacted region and introduces unreacted fluid into the reacted fluid region. At $t = 5$ the lead shock front emerges from the reacted region and is about to reach the upper boundary. When reflection occurs on the upper boundary, a hot spot appears in the upper left-hand corner of the channel, characterized by substantial local inertial confinement. This hot spot releases heat and generates compression waves that locally amplify the lead shock front. At $t = 7$, the reflected wave then re-enters the reacted region and is refracted, which induces an additional longitudinal component to the wave direction. Creation of additional longitudinal compression waves through transverse wave refraction inside the reacted fluid medium is a mechanism not present in the previous 1-D work [2, 7]. At $t = 10$ the unreacted multiply shocked region of warm fluid located $x \in [4, 15]$ has a temperature gradient in the x-direction with an average temperature $T_l \approx 2$ so that the local acoustic timescale for this fluid region is $t_{al} = l/\sqrt{T_l} = 11/\sqrt{2} = 7.8$.

Figure 1 shows when $t = 12$ and $t = 14$ this region of fluid spontaneously reacts in $t_{Hl} = 4$ time units so that the ratio of heat release time to local acoustic time is $t_{Hl}/t_{al} = 0.51$. This suggests that nearly inertially confined heating will occur [10], which is evidenced by the compression wave observed in the $t = 14$ temperature contour. The interaction of transverse waves with the walls induces a localized confinement that often results in temperature rises sufficient to form localized hot high pressure spots. This phenomena has been observed in both laboratory and numerical experiments [5, 11, 12]. Beyond $t = 14$ the entire preheated region behind the lead shock front reacts in another 4 time units and the accelerating wave propagates to the lead shock front where it emerges as an overdriven detonation wave.

For Case 2 the activation energy is the same as the previous case, but the pre-exponential factor is $B = 15$. A similar sequence of transient events occur with the exception that the localized explosion located in the upper left corner of the previous case at $t = 7$ is absent. With the smaller pre-exponential factor the peak pressure generated from original chemical explosion is only 5.5 whereas the previous case has a peak pressure of 7.5. The concomitant reduction in shock wave strength leads to much longer fluid induction times and no localized explosion occurs.

At $t = 30$, Figure 2 shows in the upper left hand corner an isolated region of reacted fluid that is separate from the primary distorted reacted fluid volume created by the initial explosion. This fluid reacted on a timescale greater than the local acoustic time and did not produce compression waves that could further increase the temperature of the reactants. Figure 2 shows that at $t = 40$ and $t = 60$ no localized explosion has occured on timescales short enough to produce compression waves. Since the current work uses the Euler equations and is only concerned with gasdynamic behavior, hot spot formation inside of a flame brush described in Ref. [6] falls outside the scope of the current work. Although detonation initiation does not occur through gasdynamic heating in this case, it may still occur through other mechanisms if phyiscal diffusion is present.

4 Conclusions

The 2-D simulations exhibit the same general gasdynamic behavior leading to detonation initiation observed in 1-D simulations. The primary difference between 1-D and 2-D is the role of transverse waves.

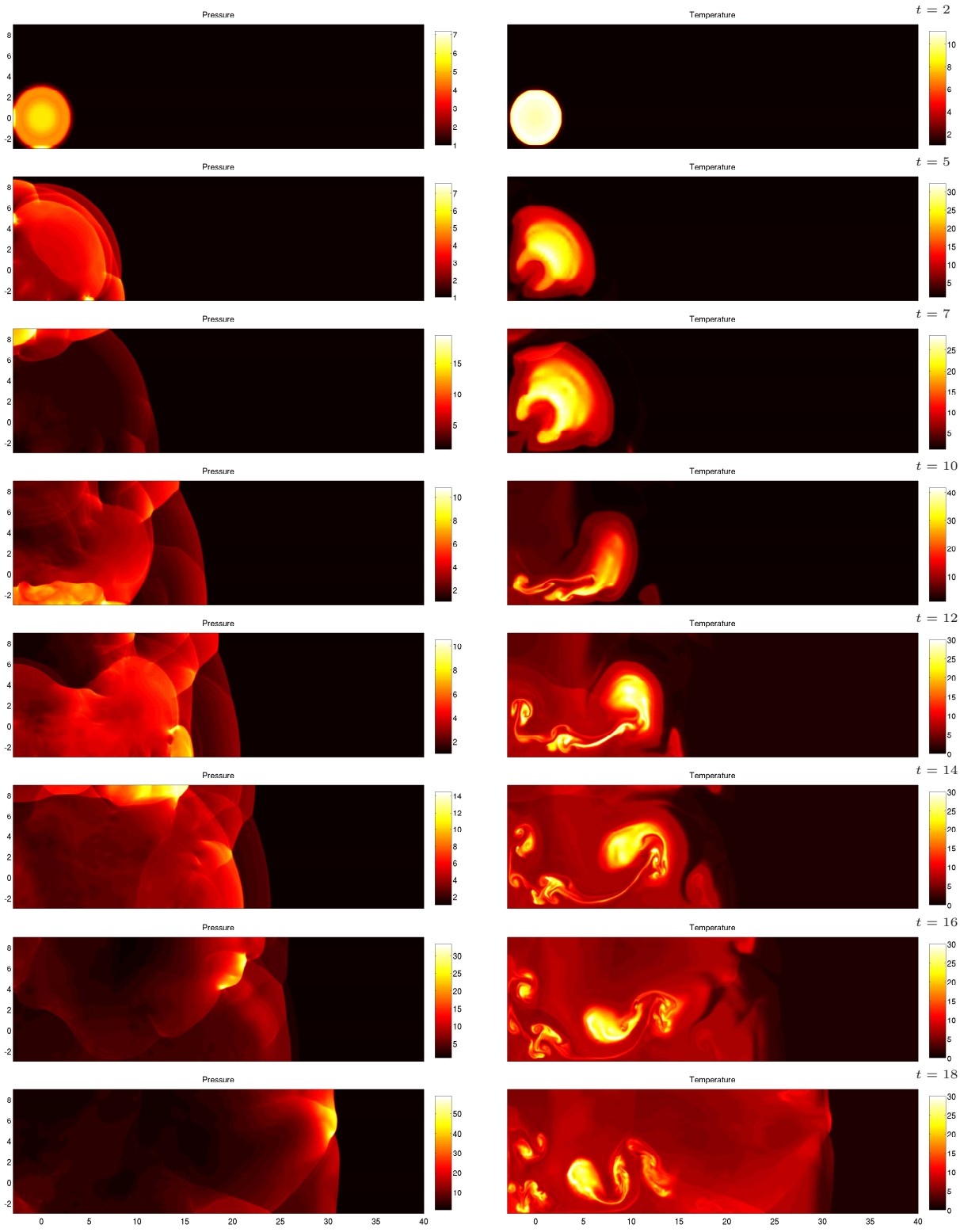

Figure 1: Pressure and temperature contour plots for output times $t = 2, 5, 7, 10, 12, 14, 16, 18$. The lead shock front decouples from the reaction zone and creates a large unreacted induction region between the reacted hot bubble and the lead shock. A spontaneous explosions occurs at $t = 14$ above the reacted bubble which accelerates until it reaches the lead shock as an overdriven detonation.

Transverse waves reflect off of the top and bottom walls and are refracted as they enter the hot products region producing successive longitudinal compression waves that can further preheat the reactants. Similar to the 1-D simulations, an induction zone of warm fluid forms and inertial confinement occurs when a localized volume of fluid spontaneously releases its chemical energy on a timescale shorter than the local acoustic timescale. The resulting compression wave accelerates through the temperature gradient until it reaches the lead shock front and produces an overdriven detonation wave.

In the case with reduced pre-exponential factor the initial explosion created by the thermal power deposition creates compression/shock waves with smaller post-shock temperatures and pressures. The reactants are heated to temperatures where the induction time is long compared to the time available in the numerical simulation. In this case, it is possible that if physical diffusion were present other DDT mechanisms that utilize turbulence may accelerate the process faster than pure gasdynamics.

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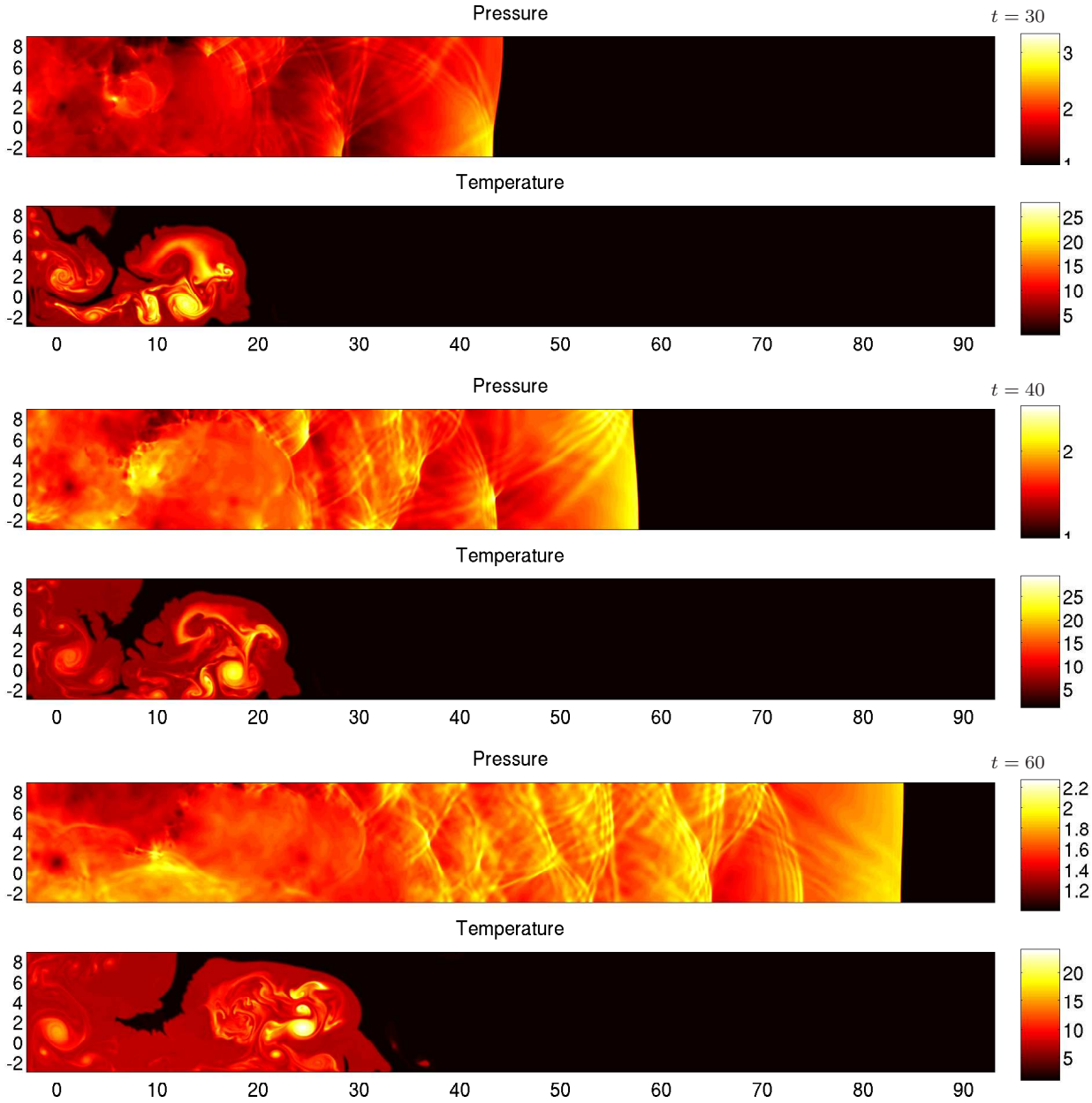

Figure 2: Pressure and temperature plots for output times $t = 30$, 40 and 60 show that detonation initiation does not occur for this case through gasdynamic processes.