Shock-initiated Ignition

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1 Introduction

Shock-initiated ignition is closely related to deflagration to detonation transition. The scenario whereby a shock moves over a slow flame, enhancing kinetics in unburnt mixture ahead of the flame can be reduced to the problem of ignition between a shock and a contact surface separating burnt (or inert) fluid from combustible mixture. This problem only lends itself to analysis under fairly restrictive conditions [1,2]. Numerically, this is a difficult problem because of the singular nature of the initial conditions. Indeed, initially, as the shock starts moving into the shocked reactive mixture, the region of interest has zero thickness. Thus, if the problem is resolved on a usual spatial grid, the domain in which the hot spot will appear and ignition will take place does not exist initially. In the absence of chemistry, the inert problem is a Riemann problem that admit the usual self-similar solution, and initially, chemistry is very slow. Thus initially the solution to the reactive problem departs from that inert solution very slowly. The difficulty associated with the singular nature of the initial conditions is eliminated when transforming the problem from using physical space x and time t as the independent variables to x/t and t, assuming that the origin $x = 0$ corresponds to the initial location of both shock and contact surface [3]. This approach yields a finite domain initially, and provides for a well resolved problem at early times and less computationally intensive simulations. The transformed problem is solved numerically using an essentially non oscillatory algorithm. Preliminary results are in good agreement with results in the literature, obtained using grid refinement. The current model yields not only the initially slow hot spot formation, but the entire process, including rapid growth of the hot spot, shock formation, retonation and the appearance of a detonation wave.

2 Physical Model

The problem is described by the reactive Euler's equations. Taking the conditions between the contact surface and the shock before chemistry occurs as the reference, we scaled pressure, density and temperature by their initial postshock values, velocity by the initial postshock speed of sound, heat release, internal energy and activation energy by the postshock speed of sound squared, and length and time in a ratio equal to the post shock speed of sound. In the transformed formulation, using the independent variable $\eta = x/t$, for single step Arrhenius kinetics, the dimensionless conservation laws become:

$$\frac{\partial(t\rho)}{\partial t} + \frac{\partial}{\partial \eta}[\rho u - \eta\rho] = 0 \tag{1}$$

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$$\frac{\partial(t\rho u)}{\partial t} + \frac{\partial}{\partial \eta}[\rho u^2 + p - \eta\rho u] = 0 \tag{2}$$

$$\frac{\partial(t\rho e)}{\partial t} + \frac{\partial}{\partial \eta}[u(\rho e + p) - \eta\rho e] = 0 \tag{3}$$

$$\frac{\partial(t\rho\lambda)}{\partial t} + \frac{\partial}{\partial \eta}[\rho u\lambda - \eta\rho\lambda] = t\rho K(1-\lambda)exp(-E/T) \tag{4}$$

Where ρ is density, u, velocity, p, pressure, e, internal energy, λ, product mass fraction, K, rate multiplier, E, activation energy and T, temperature, which is given as a function of p and ρ by the dimensionless equation of state $T = p/\rho$.

The physical initial conditions correspond to a non-reactive Riemann problem at $x = 0$. For negative x, the initial conditions correspond to unburnt mixture at a uniform state and coming from infinity at constant speed, while the positive x region is filled by burnt or inert mixture also at a uniform state and moving at constant speed. Boundary conditions at infinity match these initial conditions on both sides. In the transformed problem, and on a frame of reference attached to the initial post-shock mixture, the solution to the inert Riemann problem yields the initial conditions: the shock is located at a value η_s equal to the opposite of the shock speed in relation to the shocked mixture at rest and the contact surface is located at $\eta = 0$. In the interval between shock and contact surface, initially pressure, density and velocity $p_s = \rho_s = 1$ and $u = 0$. Since pressure and velocity are continuous across, in the region behind the contact surface, and ending at an expansion wave located at a value of η equal to the local speed of sound, their values remain equal to $p_s = 1$ and $u = 0$, but density and temperature values are determined by the solution to the Riemann problem. In the transformed frame, full resolution is available in the region between the shock and the contact surface from the beginning of the simulation, overcoming the difficulty due to non-existence of an initial physical domain and resulting staircasing effects, when solving on a regular spatial grid. The dimensionless state ahead of the shock is determined as a function of the shock Mach number using the Rankine-Hugoniot equations.

3 Numerical Simulation

The transformed problem is solved numerically using a second order accurate Essentially Non Oscillatory (ENO) scheme. The code used is an adaptation of a code first developed by Xu et al. [4], which has been parallelized using MPI (Message Passing Interface), is well-validated [5] and was significantly modified to handle the current formulation. The transformation entails changes in the CFL condition which needed to be dealt with in an appropriate manner. In the transformed variable η, initially the leading shock is located at a value η_s equal to the opposite of the speed at which the shock is moving away from the contact surface,i which is located at $\eta_{cs} = 0$. Thus the solution domain goes from a negative value of η somewhat smaller than η_s to a positive value somewhat larger than the speed of sound in the burnt (or non-reactive) mixture behind the contact surface. This guarantees that the leading shock will never reach the left boundary. Likewise, since the right boundary is placed at a value of η greater than the local speed of sound (behind the contact surface), acoustic waves originating from the reaction zone and going across the contact surface will never reach the end of the computational domain. A resolution study was performed, progressively doubling the number of grid points along η, from 6,400 to 102,400, at which point no significant difference could no longer be seen in the results.

4 Results

Results were obtained using a resolution of 51,200 grid points, for $Q = 4$, $E = 15$ and $\gamma = 1.4$. The shock Mach number $M_s = 0.70$. The density behind the contact surface was set at $\rho = \rho_B = 0.25$.

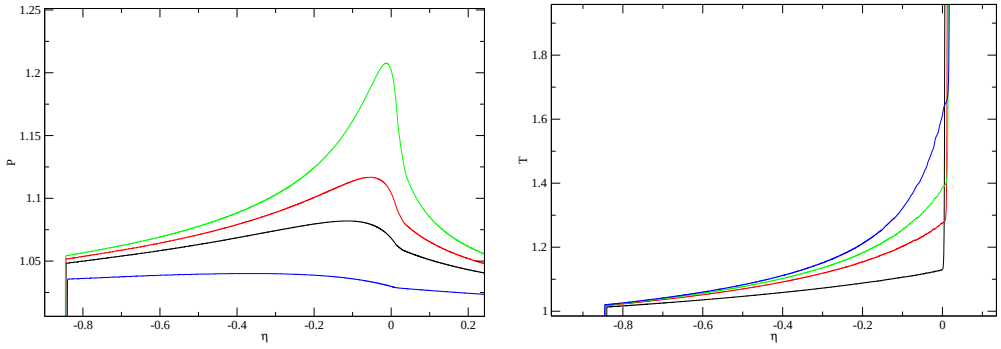

Figure 1: Early times: hot spot formation and growth at times t = 1.620, 2.044, 2.142 and 2.214. Left: Pressure profiles. Right: Temperature profiles.

Figure 1 shows the evolution of pressure and temperature during the early phase of hot spot formation. At t=1.620, the pressure maximum is located at some distance away from the contact surface. As time goes by, this pressure maximum moves closer to the contact surface, as the chemical reaction accelerates in the hot spot. The pressure maximum is closest to the contact surface when t=2.214, which is the time of the last (highest) pressure profile in Figure 1. During this initial phase, temperature increases monotonically in space from the shock to the contact surface, which is consistent with the time period since the local mixture was shocked. One also can see that the contact surface is being pushed toward the right due to the thermal expansion induced by chemistry. However the temperature maximum remains located at the contact surface during this phase.

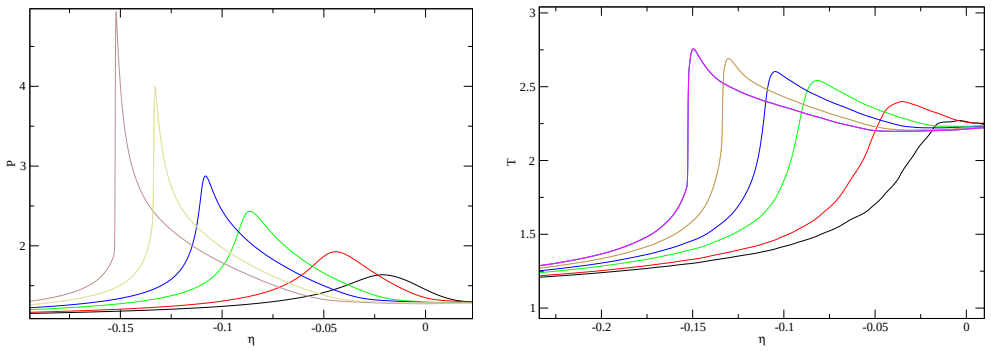

Figure 2: Later times: transition into a detonation wave at times t = 2.266, 2.286, 2.321, 2.340, 2.361 and 2.378. Left: Pressure profiles. Right: Temperature profiles.

Figure 2 shows the pressure and temperature profiles while transition into a detonation wave occurs. First the peak in pressure moves left, towards the leading shock and away from the contact surface. In Figure 2, while initially, as in Figure 1, temperature was monotonically increasing up to the contact surface, at t=2.266, an internal temperature maximum appears, moving left from the contact surface. It subsequently continues moving away from the contact surface as time evolves, closing up and eventually merging with the pressure peak. Profiles at later times show the pressure wave steepening into a new shock wave distinct from the leading shock hence appearance of a detonation wave moving toward and eventually merging with the leading shock (not shown on the figures). Before merging, this new

detonation wave continues strengthening and the peak pressure and temperature continue growing, until it encounters the leading shock, when a reflection takes place. A weaker detonation continues propagating into the colder mixture coming from left, while a retonation wave moves back.

These results are close to those of Sharpe et al. [6], validating the current formulation and its implementation. Next, the code will be used for a more thorough exploration of the parameter space, and also, using realistic chemical kinetics.

5 Conclusion

A numerical simulation of ignition between a contact surface and a shock was performed in one dimension, using a transformed coordinate system that overcomes the inherent initial singularity present in the original physical problem formulation, using an ENO scheme. In the new coordinate system, an appropriate implementation entailed a different CFL condition. Results show the complete chain of events that take place during shock ignition, from slow formation and rapid growth of the hot spot to the birth of a secondary shock and its transition into a detonation wave. Small pressure waves moving to the right behind the contact surface were also captured by our calculations. During the induction phase the pressure peak first appeared somewhere in the region between the shock and the contact surface and started to move closer to the latter, whereas in the same time interval the temperature peak remained located at the contact surface. At later times the pressure and temperature peaks started to move toward the leading shock, with the pressure peak located slightly ahead of its temperature counterpart. Eventually both of the peaks merged, as a shock formed. The current results are in close agreement with those obtained by Sharpe et al. [6]. The current model is currently being modified to handle multistep chain-branching kinetics [7-8].

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