Evolution of Stable and Pulsating Planar Detonations: Piston and Reflected Shock Initiation.

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The ignition of a detonation wave by the motion of a piston or by the reflection of a shock from the end wall of a shock tube is a subject which has received much attention, experimentally (e.g. [1,2]), theoretically [3-8], and numerically [9-11].

In order to investigate the evolution of planar detonations, initiated by a constant velocity piston or equivalently by shock reflection, extremely long time, very high resolution one-dimensional numerical simulations are performed. A hierarchical adaptive second-order Godunov scheme is used to perform the calculations. The boundary at $x = 0$ is a reflective condition, and the initial conditions are given by the quiescent (unreacted) state of the fuel, which is moving to the left at constant speed. Hence, this corresponds to a piston moving at constant speed into the initially stationary fluid, as viewed from the piston rest frame, or a reflection of a shock from a stationary wall, at the point at which the incident shock has just reached the wall. A resolution of 128 points per half-reaction length of the steady detonation corresponding to the given piston speed is used. Resolution studies are performed to show that this is about the minimum required to fully resolve the very short time and space scales involved in the ignition process and also to fully resolve large amplitude pulsating detonations. The domain size is some 32 000 half-reaction lengths. The characteristic (unit) time and length scales are taken to be the half-reaction time and length of the steady detonation.

Firstly, a single irreversible, Arrhenius reaction rate is used, since this is the most widely studied model in previous work. Parameter sets are first investigated for which the steady detonation which should ultimately be produced for a given piston speed is one-dimensionally stable. Previous work [3,4,6,10,11] is extended to much later times. As found previously, the initial stages of the evolution consist of an induction zone behind the leading shock produced by the piston motion, followed by thermal runaway at the piston, the subsequent creation of a forward moving shockless reaction wave (which consists of a quasi-steady weak detonation, unsteady combustion region, and quasi-steady fast flame [10]), the creation of a second (reaction) shock as the weak detonation slows to the Chapman-Jouguet speed and the subsequent amplification of the reaction shock and heat release rate to form a detonation. The calculations in [10] terminated shortly after the formation of the detonation. However, at this stage the detonation is still propagating through the inhomogeneous induction zone behind the leading shock.

Here, the collision of the detonation with the leading shock, and the subsequent evolution of the detonation is considered in detail. When the detonation overtakes the leading shock, a new transmitted shock (moving faster than the leading shock before the collision), a contact discontinuity and an expansion wave are created near the point of collision. The reaction zone of the detonation remains behind the contact, while the transmitted shock accelerates away from it and into the upstream, quiescent gas, igniting new reactions behind it. The new leading shock and heat release amplify each other so that the outcome is a highly overdriven detonation now propagating into the quiescent, upstream fuel. The old reaction zone behind the lagging contact eventually burns out, producing pressure waves. Indeed, many large amplitude gasdynamical disturbances downstream of the front are produced in the collision.

The now leading overdriven detonation begins to relax towards the steady state. A downstream rarefaction which overtakes the front is responsible for degrading the detonation speed (shock pressure). However, this rarefaction is very weak on the detonation scale (i.e. the length scale for decrease in pressure within the rarefaction is very large compared to the reaction length) so that the rate of decrease of the detonation speed is surprisingly slow. The rate at which the detonation speed decreases also slows as the rarefaction becomes weaker and weaker. The detonation front remains quasi-steady as it slowly relaxes.

Meanwhile the gasdynamical disturbances downstream of the rarefaction, which were created in the collision of the detonation with the leading shock, interact and evolve in a complicated way, including reflections from the piston. Figure 1 shows the pressure profile of the whole flow field at various times

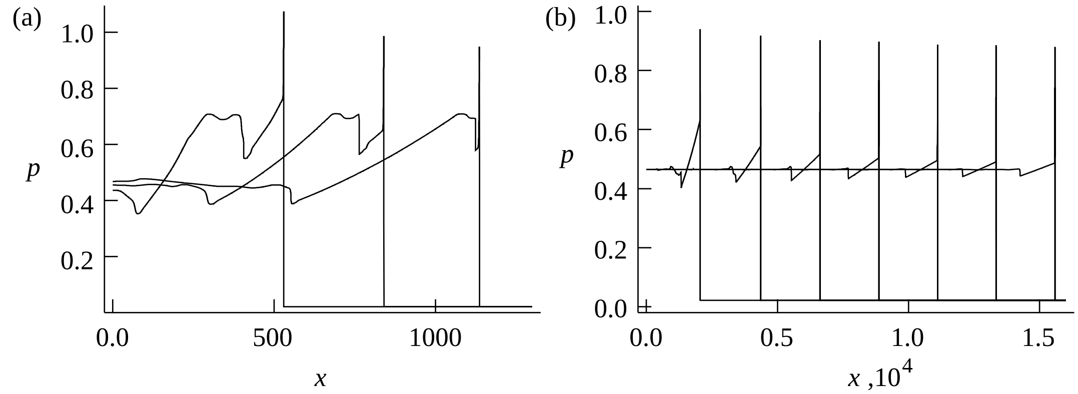

Figure 1: Pressure profiles for a one-dimensionally stable detonation at times (a) 1500, 2000 and 2500 and (b) $t = 4000$, 8000, 12000, 16000, 20000, 24000 and 28000.

after the collision. The outcome is the creation of a pair of forward moving shock waves (figure 1a). The strongest of these shocks catches up with, and eventually overtakes the detonation front, increasing the detonation speed and upsetting the relaxation process (the shock is about to overtake the front at $t = 2500$ in figure 1a). Eventually, the detonation relaxes quasi-steadily once more as the rarefaction which follows the secondary shock begins to overtake the front. However, this rarefaction is again very weak on the reaction length scale and hence the detonation speed decreases very slowly again. Figure 1b shows the pressure profiles of the flow field at several very late times. Note the very long length scale of the figure (the detonation appears as a discontinuity on this scale). The detonation speed is only within 1% of the steady detonation speed after $O(10^4)$ reaction times. Even after tens of thousands of reaction times, the complete steady state (steady detonation followed by a constant (post-detonation) state back to the piston) has not been reached. Instead, the detonation is still followed by a very weak rarefaction, which extends $O(1000)$ reaction lengths downstream. This rarefaction reduces the gas velocity below that of the piston speed at its tail, and is followed immediately by a weak shock which raises the gas velocity back up to the piston speed (figure 1b).

The effect of piston speed is then investigated and it is shown that for sufficiently high piston speed, a different formation and evolution of the detonation is found, involving the shockless reaction wave (weak detonation) overtaking the leading shock before a reaction shock can form.

Secondly, parameter sets for which the steady state is one-dimensionally unstable are considered in order to investigate the evolution of pulsating detonations. The results are compared and contrasted to calculations where the initial conditions are given by placing a steady detonation on the numerical grid (e.g. [13]). Since increasing overdrive stabilizes the detonation to the one-dimensional instability [12], the highly overdriven detonation produced in the collision of the detonation with the leading shock described above still initially relaxes quasi-steadily towards the steady state. However, the detonation speed (overdrive) begins to oscillate with a growing amplitude when the it drops below its neutrally stable value. The overdrive of the detonation is still degraded by an overtaking weak rarefaction, but on a time scale which is long compared to be a period of oscillation. Hence the pulsating detonation becomes more unstable as it propagates and the overdrive drops, and the nature of the oscillations (e.g. period and amplitude) evolve over time. Figure 2 shows the shock pressure as a function of time, for a case where the steady detonation is one-dimensionally unstable, during various time periods. For this case, calculations where the initial conditions are given by the steady detonation very quickly develop large amplitude, very irregular oscillations in the shock pressure [13]. For the piston initiated problem however, the nature of the oscillations change in time from limit cycle, through period doubling bifurcations to multi-mode, irregular oscillations as the overdrive drops and hence the detonation becomes more unstable. The nature of the oscillations eventually converges towards that of the saturated nonlinear behaviour found from calculations initiated with the steady detonation, but only on a time scale of $O(10^5)$ reaction times, or after many hundreds of oscillation periods. Note the times between bifurcations are several thousands

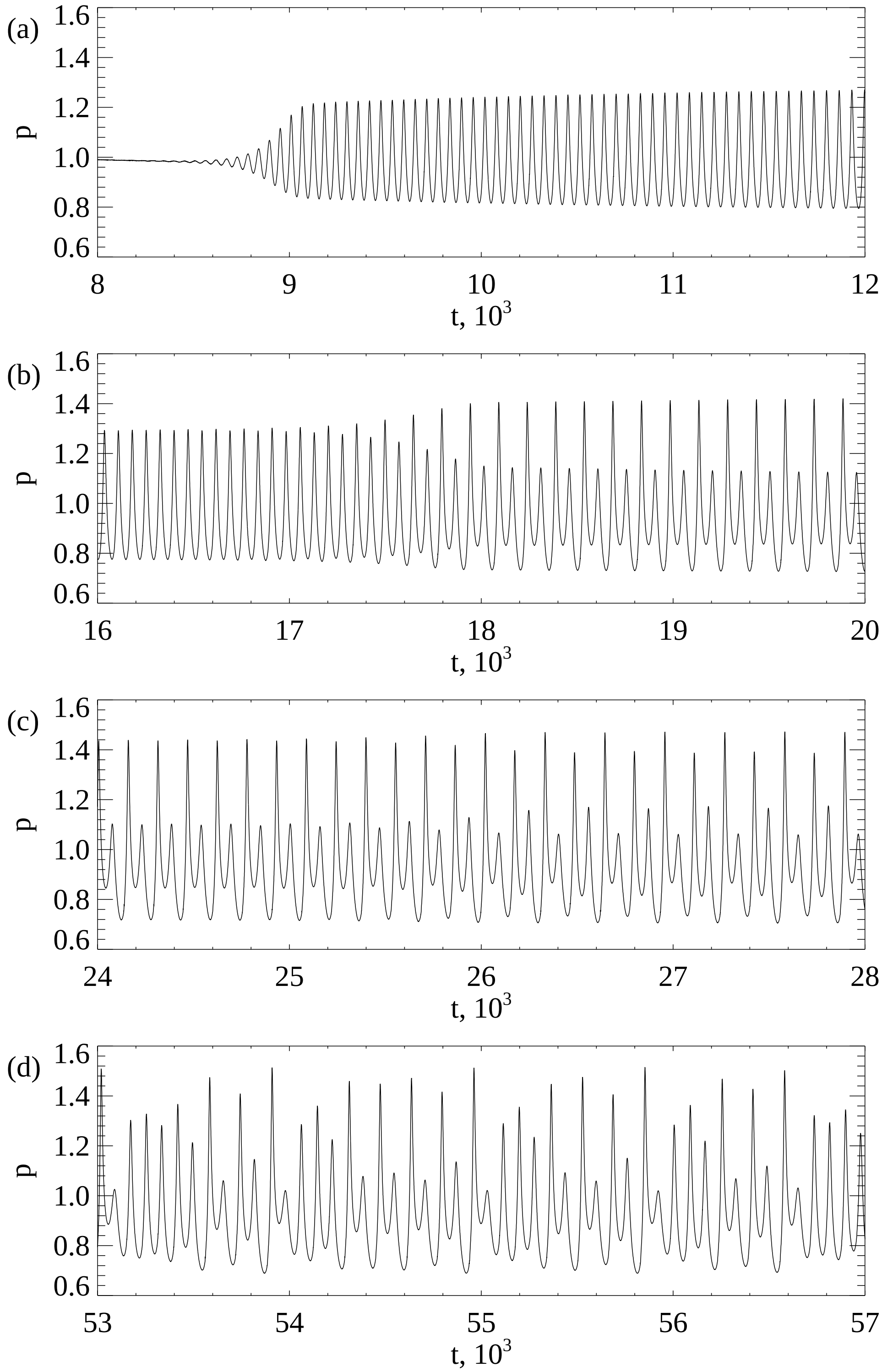

Figure 2: Shock pressure history for a one-dimensionally unstable detonation, (a) $t = 8000$ to 12000, (b) $t = 16000$ to 20000, (c) $t = 24000$ to 28000 and (d) $t = 53000$ to 57000.

of reaction times.

If one is interested in the ultimate (non-transient) behaviour of unstable detonations, these calculations highlight the need to perform very long time numerical simulations when such calculations are initiated by some unsteady (ignition) process.

Finally, since it is known that for different reaction mechanisms (e.g. chain branching), the initial stages of the piston ignition may be qualitatively different from than for the single reaction case, preliminary calculations with differing reactions (e.g model chain branching, endothermic stages of reaction, reversible reactions) will be performed in order to see if, and how, the long time evolution of the detonation differs from the single, irreversible reaction case.

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