## The Role of Cellular Structure on Increasing the Detonability Limits of Three-Step Chain-Branching Detonations

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#### 1 Introduction

In [1], the dynamics of a pulsating three-step chain-branching detonation were studied. The reaction model consists of, sequentially, chain-initiation, chain-branching and chain-termination steps. The chain-initiation and chain-branching steps are taken to be thermally neutral, with chemical energy release occuring in the chain-termination stage. The rates of each stage are given by,

$$r_I = f \exp\left(\frac{1}{\epsilon_I} \left(\frac{1}{T_I} - \frac{1}{T}\right)\right), \quad r_B = \rho f y \exp\left(\frac{1}{\epsilon_B} \left(\frac{1}{T_b} - \frac{1}{T}\right)\right), \quad r_c = y \tag{1}$$

where f is the mass fraction of fuel, and y of chain-radical. Typically,  $T_I$  is greater than the shock temperature, while the chain-initiation  $\epsilon_I$  and chain-branching  $\epsilon_B$  inverse activation energies are small. The total energy released by reaction is q = Q(1-f) - Qy. On shock passage, an exponentially small quantity of radical is produced by the exponentially slow chain-initiation mechanism. In a one-dimensional context, provided the post-shock temperature at any given time is larger than chain-branching crossover temperature  $T_b$ , the chain-branching rate constant will be exponentially large, and chain-radical mass fraction is accelerated to O(1) amounts rapidly behind the shock [1]. If the shock temperature drops to  $T_b$ , then the chain-branching rate drops to O(1) and the chain-initiation zone becomes exponentially large. For sufficiently small  $T_b$  (chain-termination zone longer than the chain-initiation zone), the ZND wave is stable. As  $T_b$  increases, the ZND solution becomes unstable, and pulsating solutions are observed. Increasingly nonlinear behavior is observed as  $T_b$  is increased further. Provided the shock temperature  $T_s$  remains above  $T_b$  during the pulsation cycles, the reaction zone and shock remain hydrodynamically coupled. However, if the shock temperature drops to  $T_b$ , it is observed numerically that the detonation shock and reaction zone will decouple, and the pulsating behavior terminates (a limit point defined as the detonability limit in [1]). For the parameter set studied in [1] and here, the shock-flame decoupled solution occurs for  $T_b \sim 0.89$ .

The structure of the 1D decoupled solution has been extensively studied in [2]. For  $T_b = 0.89$  and higher, the front pulsation drops the shock temperature to  $T_b$ . The shock amplitude then continues to decrease, the reaction zone retreats rapidly from the shock, and a decoupled shock-flame complex results. The flame propagates close to the flow velocity behind the shock; the flame zone has two spatial regions - a wide precursor zone that increases the temperature above  $T_b$ , followed by a zone of rapid chemical

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energy release. The jumps across the final shock and flame structures are close to those of an inert Riemann solution based on the quiescent upstream state and the burnt ZND solution state.

The purpose of the present study is to examine whether cellular detonation structure can increase the value of the chain-branching cross-over temperature  $T_b$  at which fully coupled detonation solutions are observed over those in 1D. The basic concept is straightforward and has been discussed in [1] and [3]; if  $T_s$  drops below  $T_b$  at the lead shock, the passage of a transverse shock can increase both the lead shock temperature and the temperature behind the transverse wave back above  $T_b$ , thus sustaining an unstable cellular detonation for values of  $T_b$  for which a one-dimensional pulsating detonation will fail. Experiments potentially supporting this hypothesis with irregular detonations have been shown in [3] in a shock tube with acoustically absorbing walls. Removal of the transverse waves results in detonation failure, giving way to a decoupled shock-flame complex. A number of questions remain to be addressed regarding the possibility of such a mechanism, and, if so, about the precise mechanisms driving the cellular structure for large  $T_b$ . For instance, one might ask what sets the cell size in a chain-branching detonation, particularly, could the characteristic cell size be set by the chain-branching cross-over temperature  $T_b$ . After a transverse wave shock collision, the strength of the transverse wave weakens as it propagates along the front. If the spacing between shock collisions is too large (cell size), then the transverse shocks may weaken to the extent that the lead shock temperature or that behind the transverse waves is not raised above  $T_b$ , losing chemical energy to drive the front in those regions. Failure may result when sufficient of the lead shock is not driven above  $T_b$  to sustain reaction.

Our starting point for generating cellular solutions is as in [1], consisting of an initial ZND wave in the channel, but perturbed here by a density non-uniformity to generate a cellular structure. Exactly how far the detonability limits (value of  $T_b$ ) can be extended is not addressed here, as such issues relate in part to the way the cellular structure is generated [6]. Our concern here is to investigate the mechanisms of self-sustained cellular detonation for values of  $T_b$  above those that lead to 1D pulsating wave failure that can be generated from the initial ZND wave. Finally, we do not consider cellular propagation driven by a process of apparent thermal ignition of hot-spots downstream, a mechanism that arises close to the 2D detonability limit. Such events are subject to the lack of correct thermal diffusive physics in the model and thus to the form of numerical dissipation in the underlying flow algorithm.

### 2 Model

The three-step chain-branching detonation model is described in [1], with a non-dimensional form based on post-shock ZND scales. The time-scale  $\tilde{t}_s$  is chosen to render the chain-termination rate constant unity, while the length-scale is the ZND post-shock sound speed times  $\tilde{t}_s$ . The development of cellular detonation is studied in a two-dimensional channel for varying chain-branching cross-over temperature  $T_b$  and channel heights h. Initially, the ZND solution is imposed across the channel in the region x < 50, with the detonation shock at x = 50. The interaction of the ZND wave with a symmetric, spatially decaying disturbance  $\rho_d$  added to the upstream density field

$$\rho_d = 0.4 \exp\left[-2\left((x-58)^2 + (y-h/2)^2\right)^{1/2}\right],\tag{2}$$

centered on (58, h/2), leads to the generation of transverse shock waves in the channel. Depending on  $T_b$  and h, a cellular detonation solution can result. All simulations presented below correspond identically with the initial ZND conditions used in [1], i.e. Q = 3,  $\epsilon_I = 1/20$ ,  $\epsilon_B = 8$ ,  $T_I = 3$ ,  $\gamma = 1.2$  and an overdrive of 1.2. The numerical method is identical to [1], extended to 2D. Simulations were run with a resolution of 80 points per half of the length of the chain-initiation region in the ZND wave. Some of the simulations were run with double the resolution to verify that no change in the underlying cellular propagation mechanism was detected. Solid channel wall conditions are applied.



Figure 1: Numerical soot foil record for  $T_b = 0.9$  and channel height h = 12. The total channel length is 600, split into three sections of 200.



Figure 2: Numerical schlieren snap-shots of cellular structure changes for  $T_b = 0.9$  and channel height h = 12 during the last cell structure shown in fig. 1. Green lines correspond to contours of  $T_b = 0.9$ , while red lines correspond to contours of y = 0.5.

### 3 Cellular Simulations

The numerically generated soot foil record for a chain-branching cross-over temperature  $T_b = 0.9$  with channel height h = 12 is shown in fig. 1. For this value of  $T_b$ , the one-dimensional pulsating solution fails. The ZND wave interaction with the density perturbation generates two transverse shock waves, that lead to the onset of cellular detonation with a one-cell solution sustained in the channel. Thus the cellular structure has extended the detonability limit of unstable solutions. Figure 2 shows numerical schlieren snap-shots of the corresponding cellular structure changes during the last foil cell structure shown in fig. 1. Figure 2(a) is just prior to the collision of transverse waves near the center of the channel. In the central region, the reaction zone has decoupled from the shock, with the contour of  $T_b = 0.9$  having dropped back to internal to the decoupled reaction zone. Behind the transverse waves, the contours of  $T_b = 0.9$  occur within the lead shock. After shock collision, strong transverse waves are generated, with strong radical production behind the lead and transverse shocks (fig. 2(b)). In front of the transverse waves, the reaction zone has decoupled from the lead shock, a mechanism that appears similar to the process of failure of 1D pulsating solutions. At the point of transverse wave collision with the walls, the contour of  $T_b = 0.9$  occurs with the lead shock, but it is evident that the reaction zone is retreating from the lead shock in the region between the transverse waves (fig. 2(c)). As the transverse waves move in from the wall, the contour of  $T_b = 0.9$  transitions to the decoupling reaction zone. Behind the transverse waves, strong coupling between the shock and reaction zone is regenerated. The cycle repeats (fig. 2(d)).



Figure 3: Numerical soot foil record for  $T_b = 0.9$  and channel height h = 24. The total channel length is 600, split into three sections of 200.



Figure 4: Numerical schlieren snap-shots of cellular structure changes for  $T_b = 0.9$  and channel height h = 24 during the last cell structure shown in fig. 3. Green lines correspond to contours of  $T_b = 0.9$ , while red lines correspond to contours of y = 0.5.

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Figure 5: Numerical soot foil record for  $T_b = 0.92$  and channel height h = 12. The total channel length is 600. Shown is the section up to 200.



Figure 6: Numerical schlieren snap-shot of cellular structure for  $T_b = 0.92$  and channel height h = 12 during the last cell structure shown in fig. 5. Green lines correspond to contours of  $T_b = 0.92$ , while red lines correspond to contours of y = 0.5.



Figure 7: Numerical soot foil record for  $T_b = 0.92$  and channel height h = 6. The total channel length is 600, split into three sections of 200.



Figure 8: Numerical schlieren snap-shots of cellular structure changes for  $T_b = 0.92$  and channel height h = 6 during the last half-cell structure shown in fig. 7. Green lines correspond to contours of  $T_b = 0.92$ , while red lines correspond to contours of y = 0.5.

The numerically generated soot foil record for  $T_b = 0.9$  and in a channel double the height h = 24 is shown in fig. 3. In larger channels, the cell size becomes less confined by the channel height. A two-cell structure is sustained for the length of the run shown. Figure 4 shows a numerical schlieren snap-shot of the corresponding cell structure across a cell cycle. The basic mechanisms are similar to that observed in fig. 2. The cellular structure consists of regions where the shock and reaction zone decouple. Propagating transverse waves are able to recouple the fronts, sustained by transverse shock collisions and collisions with the wall. Note the large decoupled zone in (b), while the upper part of (c) shows a decoupling in progress. Figures 4(d) and (e) show prominent key-stone structures created during the decoupling process [5].

The numerically generated soot foil record for  $T_b = 0.92$  and channel height h = 12 is shown in fig. 5. The soot foil shows the generation of an initially strong cellular solution after interaction of the ZND wave with the density perturbation. During the early stages of the cellular propagation, the strength of the transverse shocks is sufficient to keep  $T_b$  above 0.92 at the lead shock. At further times, the transverse shock strength weakens, and is not sufficient to keep  $T_b$  above 0.92 at the lead shock. The reaction zone decouples, while the transverse shocks die out. Figure 6 shows a numerical schlieren snap-shot of the structure for  $T_b = 0.92$  and channel height h = 12 during the last weak cell structure shown in fig. 5. The green lines correspond to contours of  $T_b = 0.92$ . The decoupled reaction zone is visible far downstream of the lead shock.

The observation above relates to that observed earlier, namely the relation of the cell-size or channel width to the propagation of detonation and the value of  $T_b$ .. The numerically generated soot foil record for  $T_b = 0.92$  and channel height h = 6, one-half of that used in fig. 5, is shown in fig. 7. In this case, by limiting the channel height, thus decreasing the time between transverse shock and wall collisions, a half-cell detonation is sustained. Figure 8 shows numerical schlieren snap-shots of cellular structure changes for  $T_b = 0.92$  and channel height h = 6 during the last half-cell foil structure shown in fig. 7. Near the start of the new half-cell, (a), the reaction zone is decoupling from the shock, but the transition to temperatures above  $T_b = 0.92$  still occurs close to or within the shock. As the transverse shock has moved one-third of the way up the channel, the post-shock state is sufficiently strong to drive y above 0.5 behind the transverse shock. By two-thirds up the channel, the contour  $T_b = 0.92$  between the transverse shock and top of the channel has fallen back to the decoupled reaction zone, but the passage of the transverse shock successfully transitions the contour  $T_b = 0.92$  back to the lead shock (fig. (b).) As the transverse shock moves down the channel, a decoupling of the reaction zone is observed. With the transverse shock about two-thirds across the channel, the reaction has decoupled from the shock between the transverse shock and the lower part of the channel (fig. (c).). The cell cycle repeats, with fig. (d) showing that as the transverse moves up the channel, the reaction zone and shock are recoupled. Note that once the shock temperature drops below  $T_b$  at the shock, the decoupling of the reaction zone and shock occurs on a very rapid time-scale, consistent with the one-dimensional failure analysis described in [2].

In the full paper, we will discuss further solutions for a variety of chain-branching cross-over temperatures  $T_b$  and channel height h. We will also compare the decoupling mechanism of the lead shock and reaction zone observed during portions of the cellular cycle to that observed in 1D. However, it is apparent that cellular detonation solutions in a mixture governed by basic chain-branching kinetics can extend the detonability limit (specifically the value of  $T_b$ ) over those observed for 1D dynamics.

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