## Spontaneous formation of strong and weak transverse waves in detonation diffraction

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In this work we identify modes of detonation diffraction that depend on the activation energy of a single-step, irreversible, Arrhenius reaction model. This study is relevant to propulsion and safety concepts concerning detonation transmission, such as in pulse detonation engines. The initial solution is a planar ZND detonation wave propagating in a channel with an abrupt area increase (corner turning problem). To examine the three different outcomes of detonation diffraction (sub-critical, near-critical and super-critical diffraction), we carry out direct numerical simulations of the reactive Euler equations with a fixed channel half-width H (normalized by the CJ half-reaction zone length). By varying the normalized activation energy  $\theta_{CJ}$  in the Arrhenius reaction term  $\exp(-\theta_{CJ}/T)$ , we find three regimes of diffraction that resemble the cases observed in experiments (Schultz 2000). The temperature T is normalized by the von Neumann value of the reference CJ detonation.

With zero or small normalized activation energy ( $0 < \theta_{CJ} \leq 1$ ), the reaction rate is essentially independent from the thermodynamic state, so that the reaction zone length is unaffected by the shock velocity. Since the reaction rate is nearly constant, the shock front will always accelerate after diffraction. We find that the transient wavefront dynamics, due to the propagation and reflection of unsteady rarefaction waves generated by the area change, die out after a distance of about 6 *H* from the corner, and that the detonation can be treated as quasi-steady, quasi-one-dimensional after that point, Fig. 1 (a). This successful detonation transmission is similar to the super-critical case that is observed in diffraction experiments. As the detonation front is diffracting, a train of weak transverse waves develops near the corner and moves toward the axis of symmetry of the channel, Fig. 1 (b). The first wave is the reflected shock that forms at the corner as a result of the adjustment to the wall boundary conditions. This shock is followed by a train of acoustic disturbances that propagate in an acoustic channel embedded in the reaction zone. Compression waves are amplified by the energy release due to the chemical reaction

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FIG. 1. Schlieren images of detonation diffraction. The red line is the locus of 95% reaction completion. Frame (a):  $\theta_{CJ} = 1$ .. Frame (b): detail of the system of transverse waves. The reference segment (bottom right corner) measures  $10 \Delta_{1/2}$ .



FIG. 2. Detonation front (schlieren image), for three different reaction rates.

and become transverse shocks at the detonation front. The newly formed contact discontinuity provides in turn a channel for the propagation of more acoustic disturbances. In this process, transverse wave spacing increases by an order of magnitude from the initial half-reaction length. This mechanism of transverse wave propagation and amplification is studied in a simpler problem where a ZND-CJ planar detonation moves in a channel over a small obstacle. Simulations of this problem show a qualitative similarity with the results obtained for the diffracting detonation (Fig. 2). The initial amplification of acoustic disturbances agrees favorably with the mechanism proposed by Strehlow and Fernandes (1965) and Barthel and Strehlow (1966).



FIG. 3. Schlieren images of detonation diffraction for  $\theta_{CJ} = 3.5$ . The red line is the locus of 95% reaction completion. Frame (a): t = 32.13. Frame (b): t = 46.77.

When the activation energy is larger,  $3.75 \ge \theta_{CJ}$ , the reaction rate is strongly dependent on the thermodynamic state so that the reaction zone length increases rapidly when the shock speed decreases. This causes the reaction zone to decouple from the shock wave, and the reaction rate to essentially drop to zero, after a short distance from the corner vertex. The detonation fails completely and the resulting flow is essentially a non-reactive shock wave. This is similar to the case of sub-critical diffraction that is observed in diffraction experiments where the tube is smaller than the critical size needed for successful detonation transmission. The shock decay rate of this case is found to be only qualitatively similar to the decay rate of a cylindrical blast.

For  $2.5 \leq \theta_{CJ} \leq 3.5$ , the reaction rate is moderately dependent on the thermodynamic state. The reaction zone length increases as the shock decays but the accelerating effects of energy release are sufficient to cause the reaction zone length to decrease in an abrupt fashion. This ultimately causes the appearance of a re-initiation event near the wall that propagates back to the axis, Fig. 3. This is similar to the case of critical diffraction that is observed in diffraction experiments where the tube is comparable to the critical size needed for successful detonation transmission. Re-initiation occurs through the interplay of transverse rarefaction waves with the accelerating detonation front near the channel axis. This results in shock folding and in the formation of a transverse shock that is kinked at a second triple point interior to the detonation, Fig. 4. Similar waves have been observed in recent simulations of cellular structures in reactive mixtures (Sharpe 2001; Inaba and Matsuo 2001). The kink is due to the high-pressure region that forms when the transverse shock processes pockets of compressed

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FIG. 4. Structure of transverse wave, contours of pressure, (a), and numerical schlieren images of density, (b). The solid line in (b) is the 0.95 reaction locus. In (a), contour lines are spaced by the non-dimensional value 2.083. A cutoff value of 250 is used (the local maximum value is 445), to mark the pressure peak position behind the kink. The segment at the bottom left indicates the length of  $\Delta_{1/2}$  in the plot scale. The two images are a close up of a frame at t = 30.30 computed for  $\theta_{CJ} = 3.5$ .

and unburnt fuel behind the partially decoupled detonation front. Multiple systems of transverse waves eventually overlap, thus enhancing the reactivity behind the leading wavefront. Where the front is completely recoupled, weak transverse waves appear with the spacing observed in the super-critical diffraction case.

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