Predicting Runaway Reaction in a Solid Explosive Containing a Single Crack

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1 Introduction

Mechanically damaged high explosive (HE) undergoing deflagration has recently [1] been shown capable of generating combustion pressures and flame speeds dramatically in excess of those observed in undamaged HE. Flame penetration of HE cracks large enough to support the reaction zone serves to increase the burning surface area and the rate of gas production. Cracks confine the product gas, elevating the local pressure and reducing the reaction zone thickness such that the flame can enter smaller-width cracks. As the reaction zone decreases sufficiently to enter the smallest cracks, the flame surface area will grow appreciably, rapidly pressurizing the cracks [2].

This runaway of pressure and burning area, termed combustion bootstrapping [2], can dramatically accelerate the combustion mode and in the most extreme cases may result in deflagration-to-detonation transition [3, 4]. The current study is intended to help predict the conditions required for the onset of reaction runaway in a narrow slot in HE. We review experiments [5] where flames were observed to propagate though a narrow slot (intended to simulate a well-formed crack) in high explosive at velocities up to 10 km/s, reaching pressures in excess of 1 kbar. Pressurization of the slot due to gas-dynamic choking is then used to predict the onset of runaway reaction. This model agrees with experimental pressure measurements of observed reaction runaway in slots.

2 Pressurization due to Gas Dynamic Choking

Consider a gap between two deflagrating HE surfaces of width w and of length L that is bounded on one side by a wall and open on the other side to a large volume of significantly lower pressure than the gap pressure P_2. Furthermore assume that the temperature inside the slot is fixed at the temperature of the reaction zone T_2 due to the large surface area to volume ratio. As shown in Fig. 1a, gas will be injected into the slot from the reacting HE and will escape from the open end of the slot. Applying the mass equation to the control volume in Fig. 1a yields

$$\frac{d\rho_2}{dt} = \frac{2\rho_2 u_2}{w} - \frac{\rho_{out} u_{out}}{L}\,. \tag{1}$$

The maximum possible gas outflow from the slot will occur when the flow is choked. Assuming isentropic choked flow with constant ratio of specific heats γ at the slot exit, Eq. 1 becomes

$$\frac{d\rho_2}{dt} = \frac{2\rho_2 u_2}{w} - \frac{\rho_2}{L}\sqrt{\frac{2\gamma_2 R_2 T_2}{\gamma_2 + 1}}\left(\frac{\gamma_2 + 1}{2}\right)^{\frac{1}{1-\gamma_2}} \tag{2}$$

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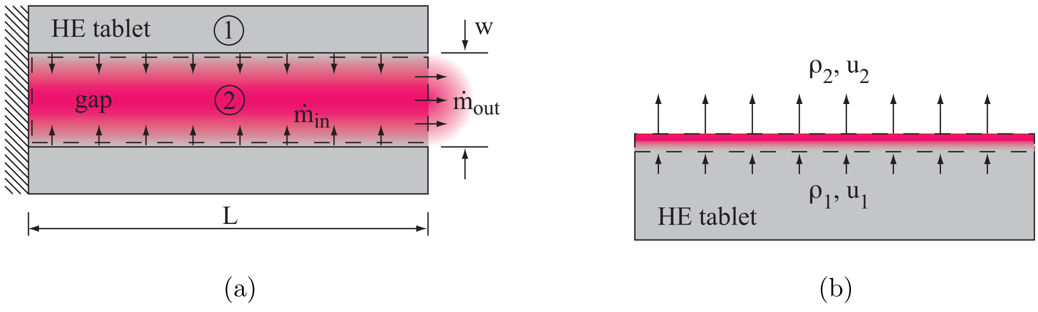


Figure 1: A sketch of (a) the control volume (dashed line) for a two dimensional slot and (b) mass flux across a control volume centered on the reaction zone of the HE.

where the gas in the slot (state 2) is assumed to be at the stagnation condition and P_{atm} is the pressure outside the slot.

The middle term of Eq. 2 can be related to the burn rate of the explosive using the mass equation ($\rho_2 u_2 = \rho_1 u_1$) applied to the reaction zone at the burning surface (Fig. 1b). Work by Maienschein and Chandler [6] has found the burn rate of PBX 9501 to be well approximated between 200 and 4000 bar by

$$u_1 = 3.4 \times 10^{-3} + 9.5 \times 10^{-10} P_2 \tag{3}$$

where P_2 is in Pa and u_1 is in m/s. Substituting the mass equation and Eq. 3 into Eq. 2 allows the mass inflow per unit area to the slot to be expressed as a function of the pressure in the slot and the initial density of the explosive. Using the perfect gas relation to then eliminate ρ_2 from the last term yields

$$\frac{d\rho_2}{dt} = \frac{2}{w}\left(3.4 \times 10^{-3}\rho_1 + 9.5 \times 10^{-10}\rho_1 P_2\right) - \frac{1}{L}\left(\frac{\gamma_2 + 1}{2}\right)^{\frac{1}{1-\gamma_2}} \sqrt{\frac{2\gamma_2}{(\gamma_2+1)\, R_2\, T_2}}\, P_2\ . \tag{4}$$

Assuming that, for slot geometries with large ratios of HE surface area to slot volume, the temperature T_2 in the slot is approximately constant at the reaction zone temperature, and approximating the product gas as a perfect gas allows Eq. 4 to be rewritten as

$$\frac{dP_2}{dt} = \frac{2R_2T_2}{w}\left(c + bP_2\right) - \frac{R_2T_2}{L} aP_2\ . \tag{5}$$

where

$$a = \left(\frac{\gamma_2 + 1}{2}\right)^{\frac{1}{1-\gamma_2}} \sqrt{\frac{2\gamma_2}{(\gamma_2+1)\, R_2\, T_2}}\ , \tag{6}$$

$$b = 9.2 \times 10^{-10}\, \rho_1\ , \tag{7}$$

and

$$c = 3.4 \times 10^{-3}\, \rho_1\ . \tag{8}$$

This result can then be integrated with the initial condition $P(t = 0) = P_0$,

$$P(t) = \left(P_0 + \frac{d}{e}\right) \exp\left(e\, t\right) - \frac{d}{e} \tag{9}$$

where

$$d = \frac{2R_2T_2}{w} c \tag{10}$$

and

$$e = \frac{2R_2T_2}{w}b - \frac{R_2T_2}{L}a \tag{11}$$

to result in an expression for the slot pressure P_2 as a function of time t only.

Figure 2a shows experimental data [5] of reaction runaway in PBX 9501 containing a single slot of width $w = 80 \times 10^{-6}$ m and length $L = 19$ cm. Curves from Eq. 9 are shown next to each experimental pressure trace measured in the slot. Representative properties of PBX 9501 and its combustion products were used to calculate Eq. 9 and the curves have been offset in time to fit each experimental trace. For the experiment, the first half of the slot was filled with propellant in order to rapidly pressurize the slot, creating a choking condition. Transducer P1 was located outside the open end of the slot and P5 was at the closed end of the slot. Transducers P3 and P4 were located 7.0 cm and 13.0 cm inside the slot, respectively. The experimental test cell failed mechanically during the test when pressures reached 1 kbar, resulting in a decrease in the measured pressure. Given the simplicity of the model, Eq. 9 agrees surprisingly well with the experimental data and provides evidence that pressurization of the slot is indeed due to the onset of gas-dynamic choking. Accounting for the viscosity of the gas in the slot would serve to further accelerate the pressurization of the slot as it hinders the movement of gas towards the exit.

3 Predicting Reaction Runaway

Violent reactions can only occur in cases where the flow of gas into the slot exceeds the outflow rate. A curve for when the outflow rate is equal to the inflow rate can be found by eliminating the mass storage variable dP_2/dt from Eq. 5 and solving for L/w,

$$\frac{L}{w} = \frac{1}{2}\frac{aP_2}{(c + bP_2)} \ . \tag{12}$$

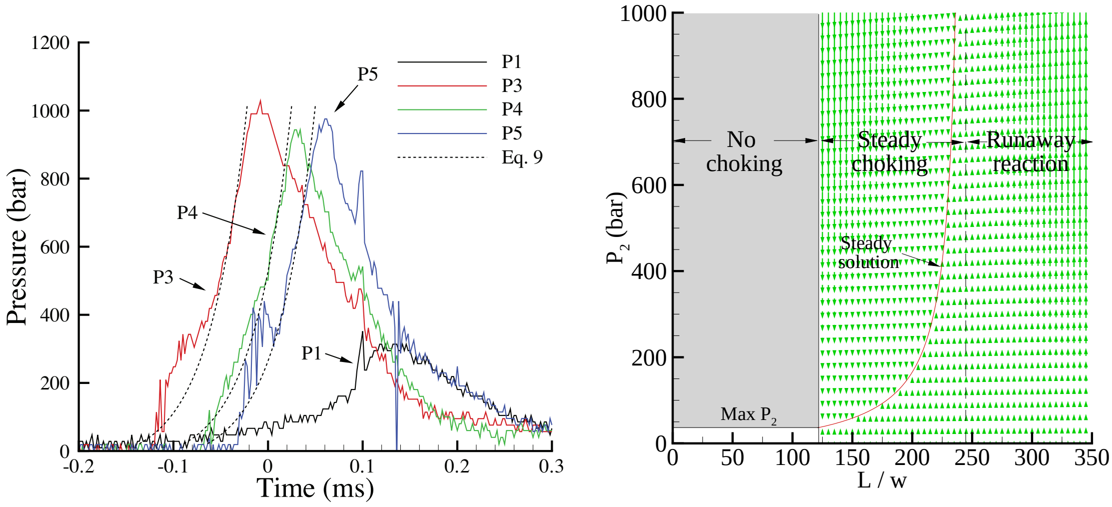
This is the steady state solution for the choked slot with mass inflow from the walls. Solutions from Eq. 9 will approach the curve described by Eq. 12 after long times.

Equation 12 is shown in Fig. 2b with three distinct regimes identified, assuming that L/w remains constant during burning. For very low values of L/w, the slot exit will not choke and the slot pressure P_2 remains below the pressure required for the onset of choking $1.8P_{atm}$. Choking occurs for values of L/w above a critical value of L/w. For a range of L/w, a balance between the inflow and outflow rates exists as described by Eq. 12 (shown in red in Fig. 2b). As indicated by the derivative (Eq. 5), all solutions in this regime move towards Eq. 12 as time progresses. The upper limit of this steady choking regime is bounded by an asymptote described by

$$\frac{L}{w} = \frac{a}{2b} \ . \tag{13}$$

For values of L/w above this asymptote, no steady state choking solution exists and the pressure continuously increases with time as indicated by Eq. 5. The region is considered the runaway reaction regime as the pressurization has no upper limit.

Comparison of this analysis to experiments [5] is of limited value due to the suspected failure of the gasket material used in the tests. For the experiments, two slot lengths, 4.06 and 19.1 cm were used and the slot width was kept constant at 80 μm. This corresponds to L/w ratios of 508 and 2388, both well into the runaway reaction regime shown in Fig. 2b, however, runaway reaction was never observed in the 4.06-cm-long-tests and was only observed in half of the 19.1-cm-long tests. Postshot disassembly revealed that gasket failure had consistently occurred in cells that did not react violently, allowing gas to vent from other portions of the slot besides the exit. This leakage is thought to have driven the solution to the left in Fig. 2b, resulting in lower pressures than expected. Nevertheless, runaway reaction did occur in half of the long slot tests. Presumably in these tests, the gasket did not fail until after the cell was destroyed by the large pressures generated. Experimental work currently underway attempts to minimize the potential for depressurization due to gasket failure and should allow better exploration of the relationship shown in Fig. 2b.



(a) (b)

Figure 2: Reaction runaway in a narrow slot. (a) Equation 9 fit to experimental traces of pressure runaway from Jackson et al. [5]. Timebases for curves from Eq. 9 are offset in time by -137, -90, and -65 μs. (b) A plot illustrating the three regimes of slot pressurization. Parameters used for calculations in both plots were characteristic of PBX 9501 properties: $\gamma_2 = 1.3$, $\rho_1 = 1830$ kg/m^3, $R_2 = 243$ m^2/(s^2 $\cdot$ K), $T_2 = 2700$ K, and $P_0 = P_{atm} = 20$ bar.

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