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PREDICTING RUNAWAY REACTION IN A SOLID EXPLOSIVE CONTAINING A SINGLE CRACK

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Abstract. This work predicts the critical conditions required for the onset of reaction runaway in a narrow high-explosive slot intended to simulate a crack. We review ongoing experiments where flames propagated through such slots at velocities up to 10 km/s, reaching pressures in excess of 1 kbar. A model is developed where slot pressurization is attributed to gas-dynamic choking at the slot exit. The combination of choking and a pressure-dependent reaction rate is shown to be capable of runaway reaction for a range of slot dimensions and pressures. This model agrees with experimental pressure measurements of reaction runaway in slots and provides a mechanism for the erratic burning observed with some explosives under high pressure.

Keywords: porosity, deflagration, PBX 9501: fracture, PBX 9501: thermal damage, confinement, cookoff
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INTRODUCTION

Mechanically damaged high explosive (HE) undergoing deflagration has recently [1] been shown capable of generating combustion pressures and flame speeds 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, resulting in rapid pressurization [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]. This study predicts the conditions required for reaction runaway in a narrow HE slot. We review experiments [5] where flames were observed to propagate through a narrow crack in HE 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 and compared to experiment.

PRESSURIZATION DUE TO CHOKING

Consider a two-dimensional gap of width w and of length L located between two deflagrating HE surfaces (Fig. 1). The gap is bounded on one side by a wall and open on the other side to a large volume of significantly lower pressure than the average gap pressure P. Gas is injected into the slot from the reacting HE and escapes from the open end. Applying

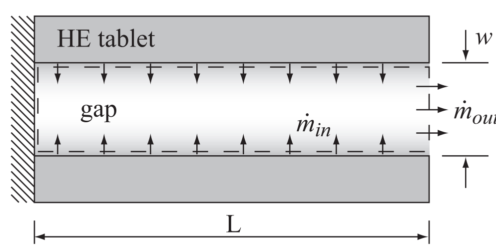

FIGURE 1. A sketch of the control volume (dashed line) for a two-dimensional slot.

the unsteady mass equation to the control volume in Fig. 1 yields

$$\frac{d\rho}{dt} = \frac{2\rho_{in}u_{in}}{w} - \frac{\rho_{out}u_{out}}{L}. \quad (1)$$

The greatest mass flux out of the slot occurs when the flow is choked. Assuming isentropic choked flow of a perfect gas at the slot exit, Eq. 1 becomes

$$\frac{d\rho}{dt} = \frac{2\rho_{in}u_{in}}{w} - \frac{\rho}{L}\left(\frac{\gamma+1}{2}\right)^{\frac{1}{1-\gamma}}\sqrt{\frac{2\gamma RT}{\gamma+1}} \quad (2)$$

where the gas properties over the length of the slot are assumed to average to the stagnation condition and carry no subscripts.

Evaluation of the middle term of Eq. 2 at the burning burning surface allows $\rho_{in}u_{in} = \rho_e u_e$, where u_e is the HE regression rate and ρ_e is the HE initial density. Movement of the control volume is neglected, which mathematically is equivalent to assuming that the reservoir gas density ρ is much less than ρ_e. This approximation is valid for lower slot pressures.

Maienschein and Chandler [6] have found the burn rate of PBX 9501 to be well approximated between 200 and 4000 bar by

$$u_e = c + bP \quad (3)$$

where $b = 9.5 \times 10^{-10}$, $c = 3.4 \times 10^{-3}$, P is in Pa, and u_e is in m/s. Thus $\rho_e u_e$ can be substituted for $\rho_{in}u_{in}$ in Eq. 2, allowing 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.

For high-aspect-ratio slot geometries, the reaction zone volume is comparable to the slot volume, and the slot temperature T can be approximated as constant at the reaction zone temperature, allowing Eq. 2 to be rewritten as

$$\frac{dP}{dt} = \frac{2\rho_e RT}{w}(c+bP) - \frac{RT}{L}aP. \quad (4)$$

where

$$a = \left(\frac{\gamma+1}{2}\right)^{\frac{1}{1-\gamma}}\sqrt{\frac{2\gamma}{(\gamma+1)RT}}. \quad (5)$$

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

$$P(t) = \left(P_0 + \frac{d}{e}\right)\exp(et) - \frac{d}{e} \quad (6)$$

where

$$d = \frac{2\rho_e RT}{w}c \quad (7)$$

and

$$e = \frac{2\rho_e RT}{w}b - \frac{RT}{L}a \quad (8)$$

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

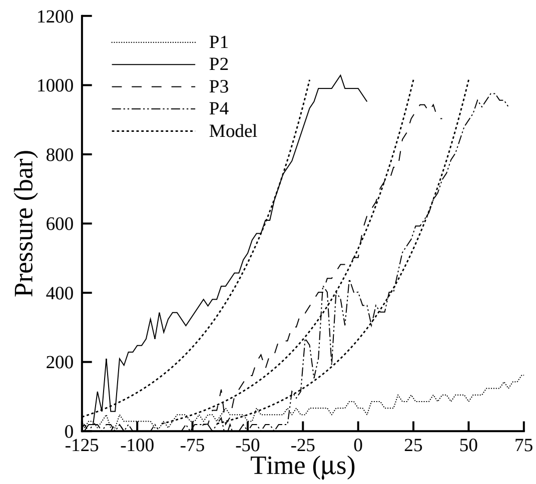

FIGURE 2. Reaction runaway in a narrow slot. Equation 6 fit to experimental traces of pressure runaway from Jackson et al. [5]. Timebases for curves from Eq. 6 are offset in time by -137, -90, and -65 μs. Traces are clipped after cell failure for clarity. Parameters used for calculations were characteristic of PBX 9501 properties: $\gamma = 1.3$, $\rho_e = 1830$ kg/m^3, $R = 243$ m^2/(s$^2 \cdot$ K), and $T = 2700$ K.

Figure 2 shows experimental data [5] of reaction runaway in PBX 9501 containing a single slot of width $w = 80$ μm, length $L = 19$ cm, and depth $d = 1.27$ cm. Curves from Eq. 6 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. 6 and the curves have been offset in time only 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 not modeled as it was located outside the open end of the slot. Transducer P4 was at the closed end of the slot. Transducers P2 and P3 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

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1 kbar, resulting in a decrease in the measured pressure. Eq. 6 agrees well with the experimental data and provides evidence that pressurization of the slot is indeed due to the onset of gas-dynamic choking.

PREDICTING REACTION RUNAWAY

Rapid pressurization 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 setting the mass storage variable dP/dt from Eq. 4 to zero and solving for L/w,

$$\frac{L}{w} = \frac{1}{2}\frac{aP}{\rho_e\,(c+bP)}\ . \qquad (9)$$

This is the steady-state solution for the choked slot with mass inflow from the walls.

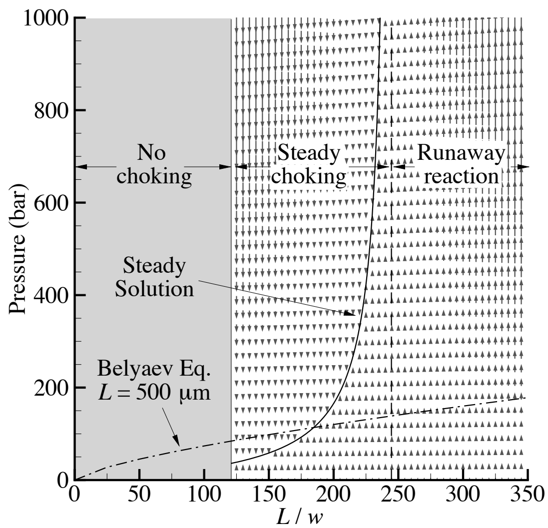

FIGURE 3. A plot illustrating the three regimes of slot pressurization. PBX 9501 parameters same as in Fig. 2.

Equation 9 is shown in Fig. 3 along with vector arrows to indicate the sign and relative magnitude of Eq. 4 at each position off of the steady-state solution. Three distinct regimes are identified. Choking only occurs for L/w above a critical value, as determined in a separate gas-dynamic analysis. For a range of L/w, a balance between the inflow and outflow rates exists as described by Eq. 9 ("steady solution" in Fig. 3). The vectors show that all solutions in this steady-choking regime move towards Eq. 9 as time progresses. The upper limit of this steady choking regime is bounded by an asymptote described by

$$\frac{L}{w} = \frac{a}{2\rho_e b}\ . \qquad (10)$$

For values of L/w above this asymptote, no positive steady-state choking solution exists and the pressure continuously increases with time as indicated by Eq. 4. 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, 4.1 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. 3, however, runaway reaction was never observed in the 4.1-cm-long-tests and was only observed in half of the 19.1-cm-long tests. Postshot disassembly revealed that gasket failure consistently occurred in cells that did not run away, 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. 3, 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. 3.

FLAME ENTRY IMPLICATIONS

Belyaev proposed a relation to predict the minimum pressure at which a flame will exist in a slot by assuming that product gas inflow heats the slot walls until Zeldovich's ignition criteria are met [7].

$$P^{1+2n}w^2 = const \qquad (11)$$

Subsequent work [8] has determined that, for PBX 9501, n = 0.92 and $const$ = 8 × 10^8 $kg^3m^{-1}s^{-6}$. Belyaev's relation is shown in Fig. 3 for L = 500 μm (corresponding to w = 4 μm at L/w = 125 and w =

1.4 μm at $L/w = 350$) representing a common crack width observed in thermally damaged PBX 9501 [9].

Burning cannot occur for pressures below Belyaev's line in Fig. 3. For values of L/w where the steady-choking solution lies below Belyaev's line, flames will be driven to extinction. For larger values of L/w, continuous burning modes are available above Belyaev's line in both the runaway-reaction regime and part of the steady-choking regime. The end effect is that, for very small, high-aspect-ratio cracks, flame intrusion does not occur until the pressure is sufficiently high for continuous burning to occur. Then the reaction quickly runs away or is driven to high steady-choking pressures capable of causing mechanical failure of the HE and most casing materials. This may contribute to the "erratic burning" observed at elevated pressures [6].

ASSUMPTIONS AND FUTURE WORK

This model is primarily intended to demonstrate the potential for gas-dynamic effects to drive runaway reaction. As such, many simplifications have been made for ease of presentation. In most geometries, the material compressibility and HE regression rate, which are neglected in this work, will act to decrease L/w as burning progresses, limiting runaway. Accounting for control volume movement due to HE surface regression results in a high pressure limit, above which runaway does not occur. These considerations are better represented by numerical simulations (currently underway) rather than direct integration. The improbability of a calorically perfect, ideal gas with a constant, pressure-independent reaction zone temperature is also acknowledged, as is the existence of a homogenous, subsonic, constant-pressure slot reservoir state. One-dimensional wave motion is a more probable mode of information propagation and is hinted at in experimental work. The effects of viscosity and varying crack width are worthy of further consideration, as is extension of these concepts to a connected network of porosity.

CONCLUSIONS

A model has been developed where runaway reaction in high explosive containing a narrow slot (simulating a crack) was attributed to gas-dynamic choking causing mass accumulation in the slot. The combination of choking and a pressure-dependent reaction rate was shown to be capable of predicting the pressure increase in the slot between two pieces of PBX 9501 explosive. The model was used to identify crack dimensions and pressure ranges where runaway reaction is likely to occur. When combined with Belyaev's relation, the model implies that, for extremely small slots, the only stable burning modes available run away to very high pressures.

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