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Initiation of stabilized detonations by projectiles

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Abstract. A high-speed projectile in combustible gas can initiate and stabilize a detonation wave under suitable conditions [1]. In this paper, numerical simulations of projectile induced detonation waves are presented. Using a one-step irreversible reaction model, the transition from shock-induced combustion to stabilized oblique detonation is observed via numerical simulations. An analysis of this transition by means of the critical decay-rate model, which considers a balance between energy-release due to reaction, and quenching due to shock-curvature, is presented.

1 Introduction

In this paper, we discuss progress towards understanding the phenomenon of detonation initiation by projectiles, inspired by the experiments of Kaneshige. In [2] different flow regimes, including both steady and unsteady shock-induced combustion and stabilized and unstable detonation initiations, are experimentally observed.

Experimentally, for a given projectile size and velocity, there exists a critical pressure threshold for a given mixture composition above which stabilized detonations are observed. An increase in pressure leads to an increase in reaction rates, reducing the length scales associated with chemistry. This transition between shock-induced combustion and detonation initiation is also observed numerically.

For the numerical results presented in this paper, a perfect-gas, single-step irreversible reaction model is used. Assume that a binary perfect-gas mixture consists of two components (A, B) having the same molecular weight, connected by the single irreversible reaction $A \rightarrow B$. Letting their heat capacities be equal (and constant), the equation of state of the mixture is

$$Pv = RT \tag{1a}$$

$$e = RT/(\gamma - 1) - \lambda q \ , \tag{1b}$$

where λ denotes the fraction of the product B, and q is the heat of the reaction. The first-order Arrhenius form is chosen for the reaction rate,

$$\frac{d\lambda}{dt} = k(1-\lambda)\exp\left(-E_a/RT\right) \ . \tag{2}$$

The thermodynamic quantities are nondimensionalized by the free-stream values P_o, T_o, ρ_o. The length scale is given by the half-reaction length $\Delta_{1/2}$, defined as the distance behind a CJ shock wave at which the progress variable $\lambda = 0.5$.

For the simulation results that follow, the reaction length scale ($\Delta_{1/2}$) is used to nondimensionalize distance, i.e., the nondimensional half-reaction length is fixed at 1. Instead of pressure, the size of the projectile, i.e., the fluid dynamic length scale, is varied. The mixture's parameters are $\gamma = 1.4$, $q = 12$ and $E_a = 15$.

Image sequences from transient simulations corresponding to the two contrasting regimes are shown in Fig 1 and Fig 2 for run R1 and R5, respectively. The half-reaction length $\Delta_{1/2}$ is indicated by the horizontal marker on the upper left-hand corner of each frame. The radius of the cylindrical projectile is nondimensionalized by the half-reaction length, 1 for run R1, and 5 for run R5. A supersonic inflow boundary condition that corresponds to an overdrive factor 2, i.e., $u = \sqrt{2}u_{CJ}$, is used. With successful initiation, the leading shock is expected to stabilize at the CJ angle $\beta = \arcsin(1/\sqrt{2}) = 45^o$.

For the solution procedure, a level-set approach is used to model the rigid cylindrical projectile over a Cartesian Eulerian mesh [5]. A steady non-reactive solution over the projectile is first sought (frames 1 through 8 of both figures), after which the chemistry source terms for the reactive Euler equations are switched on. The steady-state reactive solution is obtained by running the time-accurate transient simulations for a significant number of steps (on the order of 30,000). It can be seen that a steady-state reactive solution is attained (frames 9 through 16) by the termination time, corresponding to a simulated projectile flight distance of 500 and 1000 half-reaction lengths for run R1 (no initiation) and run R5 (successful initiation), respectively.

2 Critical decay rate model for initiation

The leading shocks and the contours of 50% and 90% reactions of the two cases are shown in Fig 3. A marker indicating the size of the half-reaction length is shown on the upper left. With the smaller projectile (Fig 3a), the reaction zone decouples from the shock front, while the shock induces supersonic combustion near the nose and becomes inert away from the projectile. With the larger projectile (Fig 3b), the reaction zone stays coupled as the shock turns from being normal to the incoming flow at the symmetry plane to the CJ angle $\beta = 45^o$.

The streamline plotted in Fig 3a is the CJ streamline for run R1. For run R5, because the leading shock approaches but does not reach the CJ angle, a representative streamline starting 30 units away from the stagnation streamline is used (Fig 3b). Kaneshige proposed that criticality depends on the balance that causes the temperature derivative (of a Lagrangian particle at the von Neumann point) of an unsupported (CJ) detonation to vanish. For our simple mixture (no mole change, constant R), the Lagrangian temperature evolution equation in natural coordinates [3] can be written, see [4] and [6], as

$$\dot{T} = \frac{T}{M^2-1}\left[\underbrace{\left(\gamma M^2 - 1\right)\dot{\sigma}}_{\text{A}} - \underbrace{uM^2\left(\gamma-1\right)\frac{\partial\theta}{\partial n}}_{\text{B}}\right] . \tag{3}$$

Equation 3 expresses the temperature derivative as a balance between reaction (term A) and streamline divergence (term B). For supersonic flows ($M > 1$), term A is positive ($\gamma > 1$) when the thermicity is positive (heat release rather than heat absorption). Term B is also positive since $\gamma > 1$, and the term $\partial\theta/\partial n$ is positive for streamtube expansion. In other words, the temperature derivative is positive when $A > B$. These two terms are plotted for the streamlines (see Fig 3) of R1 and R5 in Fig 4.

The (total) streamtube expansion ($\partial\theta/\partial n$) at the shock is the sum of a component due to reaction $\dot{\sigma}$ and a component due to shock curvature κ. Assuming that the curvature κ of the shock is known, the Lagrangian temperature derivative of Eq. 4 can be specialized

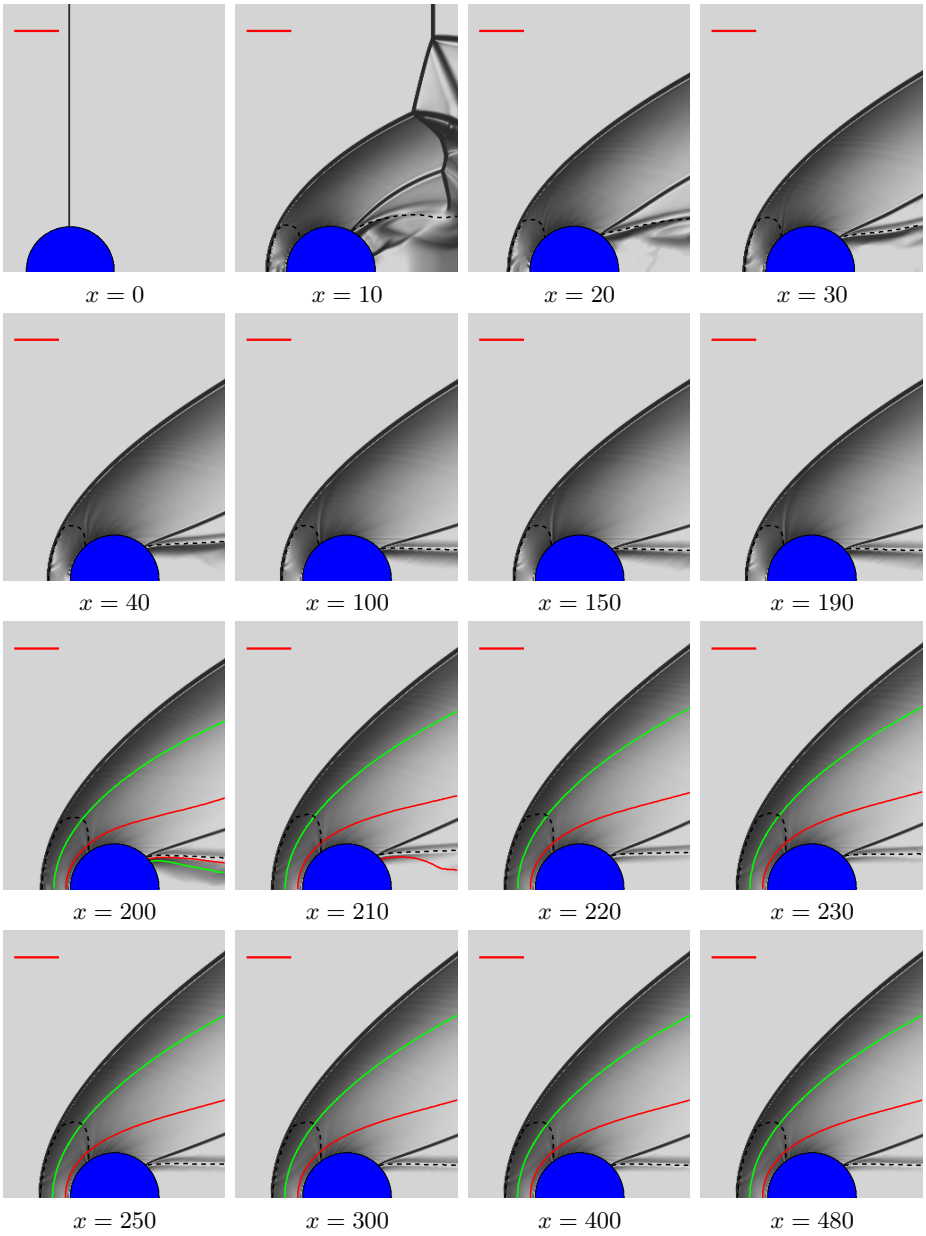

Fig. 1. Numerical Schlieren and reaction contours for run R1, zoomed in around the projectile. The black dashed line is the sonic locus.

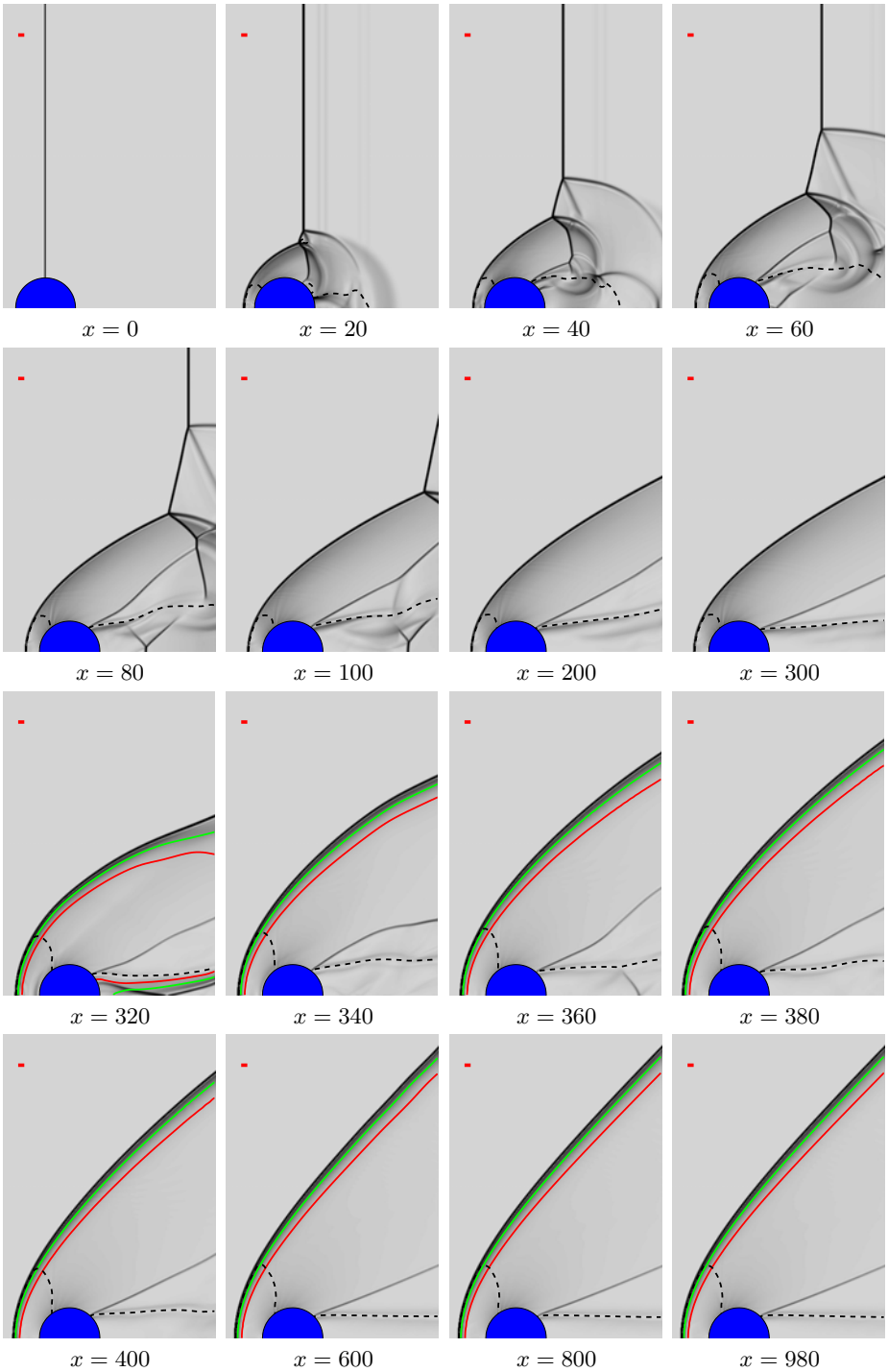

Fig. 2. Numerical Schlieren and reaction contours for case b16. The black dashed line is the sonic locus.

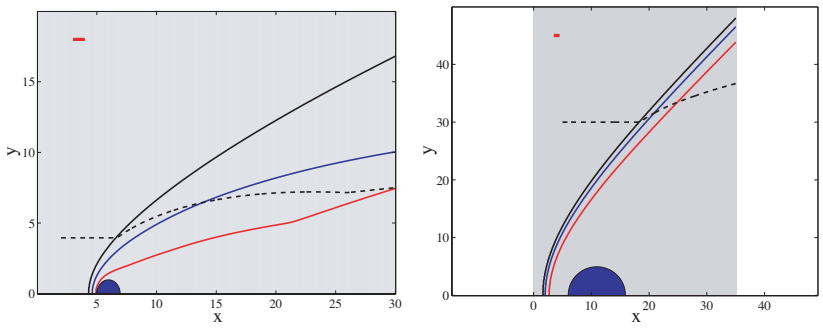

Fig. 3. Steady reactive flows over supersonic projectiles. The leading shock and contours of 50% and 90% reaction for the two cases are plotted.

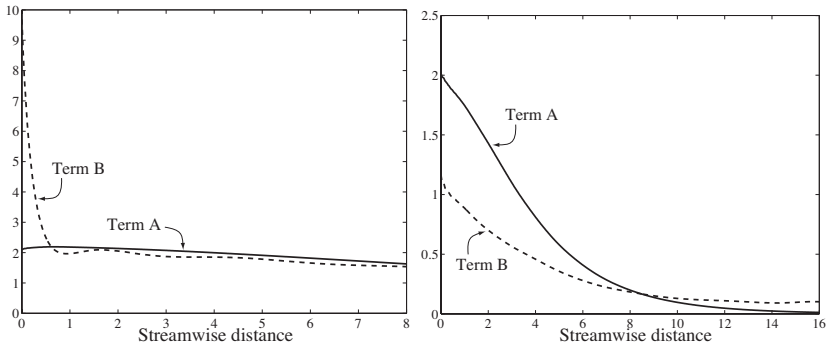

Fig. 4. Balance of heat release and expansion, see Eq. 3

at the shock to

$$\frac{\dot{T}}{T} = \underbrace{\left(1-\gamma M^2\right)\frac{\dot{\sigma}}{\eta}}_{\text{heat release}} \underbrace{- M^2\left(1-\gamma\right)\frac{\cos^2(\beta-\theta)}{\eta_n}\frac{\dot{\sigma}}{\eta}}_{\text{obliquity}} \underbrace{- M^2\left(1-\gamma\right)\frac{u}{\eta}S_2\kappa}_{\text{curvature}}, \tag{4}$$

where

$$S_2 \equiv \frac{\rho_o}{\rho}\frac{\eta}{M^2}\left\{\frac{2\cos(\beta-\theta)}{\gamma+1}\left[\frac{\cos\theta}{\sin(\beta-\theta)\cos\beta} - \frac{8}{\gamma+1}\frac{\sin\beta\cos^2(\beta-\theta)}{\sin\theta\sin(\beta-\theta)}\right]\right\} . \tag{5}$$

Equations 4 and 5 express the Lagrangian temperature derivative of a fluid particle at the shock as a function of the EOS, flow conditions, and the shock curvature. A knowledge of the latter completes Eq. 4, and, thus, the critical decay-rate model. In [6], such closure is provided by fitting the non-reactive shock profile, and the curvature is obtained by differentiation. With κ now a function of the projectile radius, setting the RHS of Eq. 4 to zero and solving gives the critical radius as a function of flow and state properties. This is plotted as a function of the nondimensional activation energy in Fig. 5. For runs R1 and R5, $E_a/RT_{vN} = 3.32$ and the critical radius under this model is predicted to be 1.7. Simulations performed with a projectile radius of 2 (not shown, see [6]) were observed to exhibit successful detonation initiation.

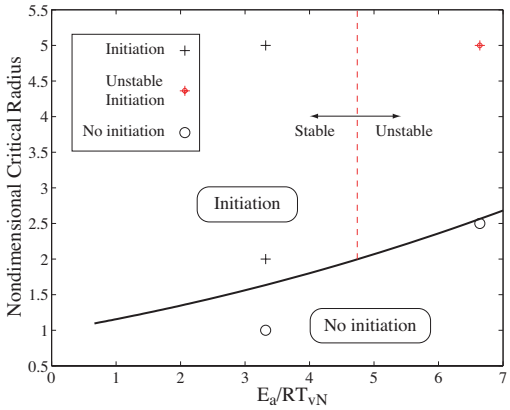

Fig. 5. Critical radius based on the critical decay-rate model as a function of E_a/RT_{vN}.

3 Conclusions

Numerical simulations of detonations initiated by hypervelocity projectiles were presented. Using a one-step irreversible reaction model, the transition from shock-induced combustion to stabilized oblique detonation was observed. Using the critical decay-rate model of [1], an analysis of this transition was presented and its prediction compared against the numerical results.

While the critical-decay rate model reconciled with the numerical experiments presented, the predicted transition at a nondimensional critical radius of ≈ 2 is some $15 \sim 50$ times smaller than experimentally observed in [2]. Sources of this discrepancy include the use of a first-order one-step Arrhenius model for reaction, a cylindrical (rather than spherical) projectile, and mixture conditions chosen to suppress transverse detonation waves. Numerical simulations using detailed reaction kinetics with sufficient grid-refinement to capture the nuances of three-dimensional detonation instabilities will be extremely challenging and require substantial advances in computational power and algorithms.

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