Prediction of the Critical Curvature for LX-17 with the Time of Arrival Data from DNS

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1 Abstract

We extract the detonation shock front velocity, curvature and acceleration from time of arrival data measured at grid points from direct numerical simulations of a $45mm$-radius rate-stick lit by a disk-source, with the ignition and growth reaction model and a JWL equation of state calibrated for LX-17. We compute the quasi-steady (D, κ) relation based on the extracted properties and predicted the critical curvatures of LX-17. We also proposed an explicit formula that contains the failure turning point, obtained from optimization for the (D, κ) relation of LX-17.

2 A direct numerical simulation of detonation initialization / propagation

The theory of detonation shock dynamics (DSD) predicts that a relationship between the detonation normal velocity D and the detonation front curvature κ, i.e. the (D, κ) relation that governs the evolution of a quasi-steady detonation. For a HE material with a large activation energy (such as LX-17), a critical curvature exists and there is no quasi-steady detonation possible with a curvature greater than this critical (failure) value [1]. In addition, the DSD theory also predicts another critical curvature such that a steady detonation cannot be initialized by a source with a radius of curvature smaller than another critical value [2]. However, to the best of our knowledge, no experimental measurement of the failure curvature has been reported with a definite conclusion, presumably because of technique difficulties associated with measurement of large curvature near the boundary of a rate-stick [3].

A direct numerical simulation by ALE3D of a $45mm$-radius rate-stick (fig. 1)is performed with the ignition and growth rate-model [4] (a well established one), and a JWL equation of state [5] calibrated for LX-17. The detonation is lit by a LX-17 disk with a 0.1mm thickness and an initial velocity of $0.75cm/\mu s$ toward the positive $x-$direction. We compute the detonation shock front velocity, curvature and acceleration from time of arrival data measured at grid points with finite difference schemes. We then look for intersections between grid-lines and the zero-acceleration contours and compute a (D, κ) pair with a linear interpolation

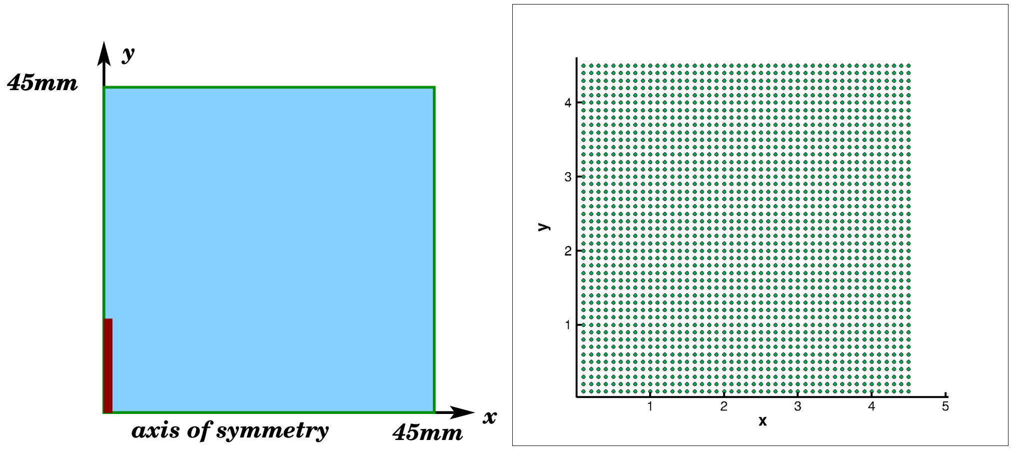

Figure 1: Left: the problem setup: the blue region is LX-17 at rest; the red disk is the detonation source (also LX-17) that has a radius of $1.25cm$ and a thickness of $0.1cm$, with an initial velocity of $0.75\ cm/\mu s$ moving in the x-direction. The axis of symmetry is $y = 0$. Right: the locations of tracers where the shock arrival time is recorded. The spacing between neighbor tracers is $h = 0.1cm$.

at each of the intersections. The result displays a clear (D, κ) relation with two turning points as predicted with the DSD theory. Thus we have found a method to predict the critical curvatures from DNS data.

3 The curvature, the normal velocity and the acceleration with a Cartesian grid

The curvature

The time of arrival $T(x, y)$ data are measured at tracers uniformly distributed on a Cartesian grid with a cell-size $h = 0.1cm$. A detonation front is defined by the function $T(x, y) = constant$. From differential geometry, the front-curvature is determined by $\kappa = \vec{\nabla} \cdot \hat{n}$, where $\hat{n} \equiv (n_x, n_y)$ is the front normal unit vector defined by

$$\hat{n} \equiv \frac{\vec{\nabla} T(x,y)}{|\nabla T(x,y)|}, \tag{1}$$

where

$$\vec{\nabla} T(x,y) = (\frac{\partial T}{\partial x})\hat{\imath} + (\frac{\partial T}{\partial y})\hat{\jmath}, \qquad |\nabla T(x,y)| = \sqrt{(\frac{\partial T}{\partial x})^2 + (\frac{\partial T}{\partial y})^2}. \tag{2}$$

Using a central difference scheme, at grid point (i, j), one has

$$\frac{\partial T}{\partial x} = \frac{T(i+1,j) - T(i-1,j)}{2h} + h.o.t.,$$
$$\frac{\partial T}{\partial y} = \frac{T(i,j+1) - T(i,j-1)}{2h} + h.o.t.. \tag{3}$$

Here, 'h' is the distance between neighboring grid lines and '$h.o.t.$' stands for '*higher order terms*'. Then it is explicit to express the curvature as (because the problem has a cylindrical symmetry, there is an additional term to the planar divergence operator)

$$\kappa = \vec{\nabla} \cdot \hat{n} = \frac{\partial n_x}{\partial x} + \frac{\partial n_y}{\partial y} + \frac{n_y}{y}. \quad (4)$$

or

$$\kappa = \frac{\frac{\partial^2 T}{\partial x^2}(\frac{\partial T}{\partial y})^2 + \frac{\partial^2 T}{\partial y^2}(\frac{\partial T}{\partial x})^2 - 2\frac{\partial^2 T}{\partial x \partial y}(\frac{\partial T}{\partial x})(\frac{\partial T}{\partial y})}{|\nabla T|^3} + \frac{\frac{\partial T}{\partial y}}{y|\nabla T|}. \quad (5)$$

The second derivatives of the arrival time at grid point (i, j) are computed as the following

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T(i+1,j) - 2T(i,j) + T(i-1,j)}{h^2}, \quad \frac{\partial^2 T}{\partial y^2} \approx \frac{T(i,j+1) - 2T(i,j) + T(i,j-1)}{h^2}$$
$$\frac{\partial^2 T}{\partial x \partial y} \approx \frac{T(i+1,j+1) - T(i+1,j-1) - T(i-1,j+1) + T(i-1,j-1)}{4h^2}. \quad (6)$$

The normal detonation velocity

By definition, the normal detonation velocity is (let s be a distance increment in the normal)

$$D \equiv \lim_{s \to 0} \frac{s}{T(x + sn_x, y + sn_y) - T(x, y)} = (\frac{\partial T}{\partial x} n_x + \frac{\partial T}{\partial y} n_y)^{-1}, \quad (7)$$

The acceleration

Also by definition, we have the normal acceleration

$$a \equiv \lim_{s \to 0} \frac{D(x + sn_x, y + sn_y) - D(x, y)}{T(x + sn_x, y + sn_y) - T(x, y)} = D(\frac{\partial D}{\partial x} n_x + \frac{\partial D}{\partial y} n_y), \quad (8)$$

where (with some algebraic manipulations)

$$\frac{\partial D}{\partial x} = -D^2 n_x \left(\frac{\partial T}{\partial x}\frac{\partial n_x}{\partial x} + \frac{\partial^2 T}{\partial x^2} n_x + \frac{\partial T}{\partial y}\frac{\partial n_y}{\partial x} + \frac{\partial^2 T}{\partial x \partial y} n_y \right),$$
$$\frac{\partial D}{\partial y} = -D^2 n_y \left(\frac{\partial T}{\partial x}\frac{\partial n_x}{\partial y} + \frac{\partial^2 T}{\partial y^2} n_y + \frac{\partial T}{\partial y}\frac{\partial n_y}{\partial y} + \frac{\partial^2 T}{\partial x \partial y} n_x \right). \quad (9)$$

Some new terms appear and are evaluated as the following

$$\frac{\partial n_x}{\partial x} = (\frac{\partial^2 T}{\partial x^2}(\frac{\partial T}{\partial y})^2 - \frac{\partial^2 T}{\partial x \partial y}\frac{\partial T}{\partial x}\frac{\partial T}{\partial y})/|\nabla T|^3, \quad \frac{\partial n_x}{\partial y} = (\frac{\partial^2 T}{\partial x \partial y}(\frac{\partial T}{\partial y})^2 - \frac{\partial^2 T}{\partial y^2}\frac{\partial T}{\partial x}\frac{\partial T}{\partial y})/|\nabla T|^3,$$
$$\frac{\partial n_y}{\partial x} = (\frac{\partial^2 T}{\partial x \partial y}(\frac{\partial T}{\partial x})^2 - \frac{\partial^2 T}{\partial x^2}\frac{\partial T}{\partial x}\frac{\partial T}{\partial y})/|\nabla T|^3, \quad \frac{\partial n_y}{\partial y} = (\frac{\partial^2 T}{\partial y^2}(\frac{\partial T}{\partial x})^2 - \frac{\partial^2 T}{\partial x \partial y}\frac{\partial T}{\partial x}\frac{\partial T}{\partial y})/|\nabla T|^3. \quad (10)$$

4 Analysis of the solution fields

The planar ZND velocity consistent with the ignition and growth model [4] and JWL equation of state [5] used in the simulation is: $D_{CJ} = 0.7696(cm/\mu s)$. Based on the DSD regularity-condition [6] a self-sustained diverging detonation must have $D < D_{CJ}$ as the curvature $\kappa > 0$. There is no quasi-steady (i.e. with zero-acceleration) detonation associated with a converging front and this is consistent with our simulation. The solution fields of shock-arrival time, curvature, velocity and acceleration are shown below in (figs. 2).

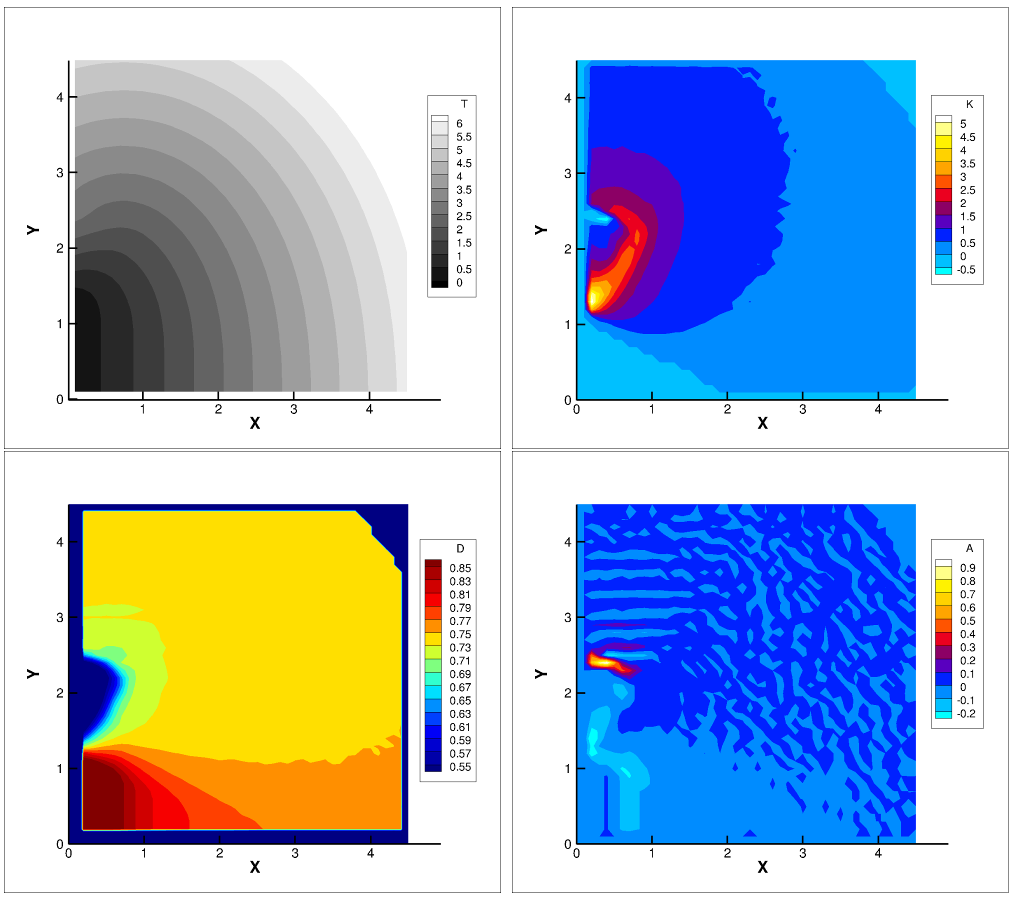

Figure 2: Upper-left: the time of arrival; upper-right: the curvature field; lower-left: the velocity field; lower-right: the acceleration field.

The region of initialization

The region with $D > D_{CJ}$ shown in the lower left of (figs. 2) is over-driven (caused by the compression from the fast moving disk-source), not self-sustained. In fact, the detonation there is not quasi-steady, otherwise its intersection with the positive curvature region would have $D < D_{CJ}$. Therefore, we conclude the region $D > D_{CJ}$ is still under initialization.

A region of a dead-zone

A region with high front curvature and low detonation speed (way below the failure velocity of LX-17) appears near the bottom (with small x-coordinates) and the acceleration field there displays some pulsating behavior. From the above figures we clearly see a small negative curvature region associated with negative accelerations. We think the information contained in the arrival time there can help us to enhance the understanding of the dynamics of an unsteady detonation at a low velocity.

A region of a self-sustained diverging detonation

The rest of the computational domain can be considered as propagated through by a self-sustained diverging detonation. The acceleration there has small magnitudes and is varying around zero. We compute the intersections of the zero-acceleration contours and the grid lines and obtain interpolated values of (D, κ) on these intersections (a zero-acceleration point is linearly interpolated on an edge of a cell if its edge nodes have different signs of accelerations).

5 The turning points on the steady (D_n, κ) curve and the critical curvatures for LX-17, with a fitting formula

We observed (see fig. 3, left) from a numerical simulation the two turning points previously predicted by the DSD theory ([1], [2]). From DNS of this *disk-lighting* problem, the (D, κ) data for the entire valid curvature region is generated. In contrast, a DNS of a steady rate-stick front can only provide (D, κ) data for smaller curvatures.

Therefore, we obtained the failure curvatures for LX-17 from a direct-numerical simulation. The value of the radius of failure curvature is $\kappa_{fail} = 2.78cm^{-1}$, associated with a failure velocity with the value $D_{fail} = 0.672(cm/\mu s)$. The critical radius for initialization is about $\kappa_{init} = 0.5cm^{-1}$ at $D_{init} = 0.48(cm/\mu s)$. We can fit the (D, κ) pairs obtained above with an analytic formula with three constraints that (a). $\kappa = 0$ at $D = D_{CJ}$; (b). $\kappa = 1/r_{fail}$ at $D = D_{fail}$; (c). $\partial\kappa/\partial D = 0$ at $D = D_{fail}$. We used LX-17 rate-stick fronts from DNS with a tracer density higher than in (figs. 1) to fit a formula for the steady (D, κ) relation

$$\kappa = \kappa_c \left(\frac{1-d}{1-d_f}\right)^A exp[-B((s-d)^C - (s-d_f)^C)], \qquad (11)$$

where $\kappa_c \sim 2.78cm^{-1}$ is the critical curvature at the failure turning point, $d \equiv D/D_{CJ}, d_f \equiv D_{fail}/D_{CJ}$, $s = d_f + [(A/(BC(1-d_f))]^{1/(C-1)}$. The values of the dimensionless parameters are $A = 1.3, B = 23.0, C = 1.75$, obtained from a carpet search for optimization.

A validation of the critical curvature / velocity for LX-17

The critical curvature (and velocity) is material dependent only (in theory). To verify this, we varied the radius of the source disk from $1.25cm$ to $0.625cm$ and $2.5cm$. Similar behavior with (D, κ) are observed in each case and the locations of the turning point change little (figs. 3, right).

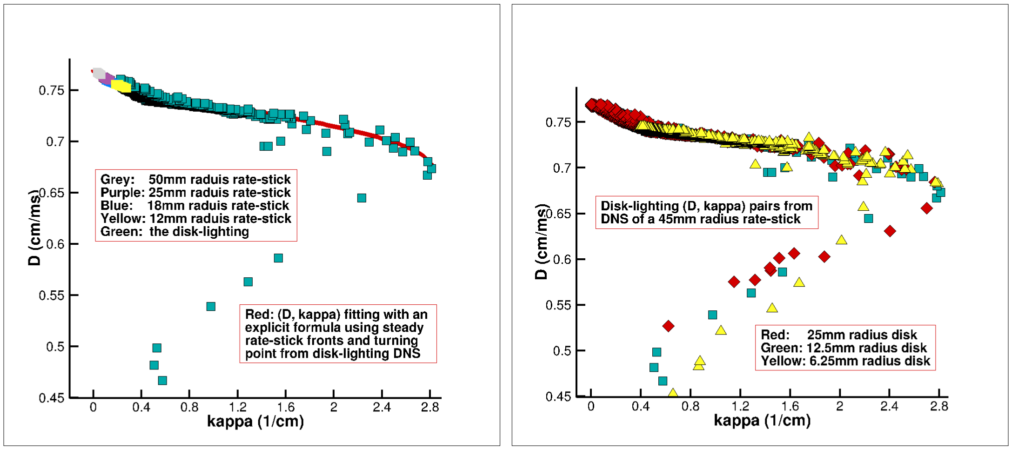

Figure 3: Left: the (D, κ) pairs extracted from the simulation with a disk-source with a radius $1.25cm$, and fitted with an analytic formula (the red curve) using steady rate-stick front geometries; right: similar (D, κ) pairs obtained with three different source radii. Their turning points share nearly the same location.

6 Conclusion

We evaluate the acceleration, normal velocity and curvature fields based on the time of arrival data distributed on a grid in an axi-symmetrical space obtained from a DNS simulation of a detonation that is initialized with a disk-source with a $45mm$-radius rate-stick. We extracted the steady (D, κ) pairs from the field data and the result provides a prediction of the failure curvature/velocity of LX-17.

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