Planar Blast Initiation of Detonations Using a Simplified Model

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1 Introduction

When a blast occurs in a reactive gas, its strong lead shock compresses the gas to high pressures and temperatures. The initially negligible effects of chemical reactions at early times become more important as the blast strength decays over time due to expansion. Whether a detonation is initiated or not, depends on the reactive mixture and the amount of energy deposited to create the initial blast. If the blast energy is sufficient (supercritical), a steady or pulsating detonation is directly initiated. When the blast is weaker (critical), it decays to a quasi-steady period of minimum speed, as low as 50% to 80% of the Chapman-Jouget (CJ) speed, then overshoots the CJ speed and settles back down to initiate a detonation [1, 2]. The blast decay is caused by unsteady expansion of the gas and curvature losses. If the blast energy is insufficient (subcritical), the blast fails to initiate a detonation as it decays, within a time limit. The demarcation between initiation and failure is drastic, especially in cylindrical and spherical geometries. A small decrease in blast energy leads to a very large increase in initiation distance and failure.

The objective of much research in this field is to predict the minimum blast energy required to initiate a detonation, ideally based only on the thermochemical properties of the mixture. Attempts to predict the critical blast energy have typically compared a length scale of the blast decay to a scale inherent to the mixture. Blast decay scales are often chosen as the radius when the blast has decayed to CJ or down to half of the CJ strength. The mixture length scales are associated to the induction length, detonation cell size, or other semi-empirical length scales related to propagation or initiation limits, as discussed by Lee and Higgins [1] with references therein. Though there have been many improvements since the first works, the accuracy of predictions remain on the order-of-magnitude or larger.

Due to the spherical and cylindrical nature of most blasts, the effect of curvature losses have been included in most studies. However, Lee and Higgins [1] highlighted the importance of unsteady terms by pointing out that curvature cannot explain failure in planar blasts. The significance of unsteady terms was compared to spherical curvature by Eckett et al. [2], who showed that curvature losses are less important than the

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unsteady terms in blast failure. Kasimov and Stewart [3] attributed the over-prediction of critical blast energies in their model and others', such as He and Clavin's [4], which considered curvature losses without unsteady terms, to the importance of unsteadiness and remarked that critical initiation conditions occur before critical quasi-steady curvature.

Numerical investigations of planar blasts performed by Mazaheri [5] produced supercritical and critical detonation initiation as mentioned above, but did not show as clear of a demarcation between initiation and failure at low activation energies. Subcritical blasts were defined by a decay to a near constant sub-CJ speed, later initiated by the formation of an internal shock. Planar blasts in mixtures with higher activation energies [5, 6] had a more distinct failure and did not initiate a detonation within the observed time period, as did simulations using chain branching chemical kinetics [7], but instabilities also appear to play a role in deciding if detonation initiation will occur [2, 6, 7].

The prediction of critical blast energy remains an open problem, with an order of magnitude agreement between theory and experiment in the best of cases. While previous work points to the importance of unsteady terms, stability, and choice of chemical model, the problem remains difficult to probe due to the complexity of the Euler equations. This study proposes to simplify the direct initiation problem through the use of a toy model, such as Fickett's detonation analogue [8], in order to gain further understanding on the direct initiation of detonations.

Toy models and asymptotic models of detonations were introduced by Fickett [8] and Majda [9]. They consist essentially of Burgers' equation with an added source term to mimic energy release and have seen a number of successes in reproducing detonation phenomena, from the steady structure of eigenvalue detonations [10], to pulsating instability and the period-doubling route to chaos [11, 12].

2 Model

On example of a simplified model is Fickett's detonation analogue [8], whose one-dimensional hydrodynamic equation takes the form

$$\partial_t \rho + \partial_x p = 0 \qquad \text{with} \qquad p = \frac{1}{2}(\rho^2 + Q\lambda_\mathrm{r})$$

as equation of state, where t and x are the time and space variables, ρ is the state variable, $Q = 1$ is the heat release, and λ is the reaction progress variable which ranges from zero behind the shock when unreacted to one when fully reacted. This model has two families of waves, forward-travelling characteristics travelling at a speed ρ, and stationary particle paths along which energy is released. The model lacks the rear-facing characteristics and strong non-linearities of the Euler equations while maintaining important dynamics of compressible flows.

The hydrodynamic model must be coupled to a chemical model for the energy source. The majority of direct initiation investigations using the Euler equations have simplified the chemistry to a one-step Arrhenius reaction. Many choices for chemical model are possible; for example, a two-step induction-reaction can be chosen to approximate the chemistry, consisting of a neutral induction period (no heat release) with an Arrhenius rate dependent on the instantaneous shock speed beginning at the shock, followed by fixed-rate exothermic reaction, or "fire", that begins once the induction period is complete. The induction and reaction rates considered in this paper (subscripts i and r, respectively) are

$$r_\mathrm{i} = \frac{\mathrm{d}\lambda_\mathrm{i}}{\mathrm{d}t} = \mathrm{H}(1-\lambda_\mathrm{i}) \exp\left(E_\mathrm{a}\left(\frac{D}{D_\mathrm{CJ}} - 1\right)\right) \quad \text{and} \quad r_\mathrm{r} = \frac{\mathrm{d}\lambda_\mathrm{r}}{\mathrm{d}t} = (1 - \mathrm{H}(1-\lambda_\mathrm{i}))k(1-\lambda_\mathrm{r})^\nu \qquad (1)$$

where H is the Heaviside function, E_a is the activation energy, D is the shock front speed equal to $D_\mathrm{CJ} = \sqrt{Q}$ at steady-state, k is the reaction rate prefactor, proportional to the ratio of induction and reaction lengths, and $\nu = 1/2$ is the reaction order. The stability of this chemical model in Fickett's detonation analogue has previously been presented by Bellerive et al. [13–15], and depends on both the activation energy and the reaction rate prefactor k, which controls the ratio of induction and reaction lengths. Stable, pulsating, and chaotic detonations are possible.

3 Methodology

The system of equations were solved numerically in the shock-fixed frame of reference using a second order Godunov scheme with a minmod flux limiter and an extrapolation outflow. A resolution of 200 points per steady state induction zone length was used, and the time step size was selected using the Courant-Friedrichs-Lewy condition with $\mathrm{CFL} = 0.8$.

The flow was initialized to approximate the blast decay at an early time $t_0 = 10^{-3}$ with an expansion wave connected to the shock front such that

$$\rho(x,t_0) \approx \begin{cases} 0 & \text{if } x_\mathrm{s} < x \\ \max\left(\frac{2D_0}{x_\mathrm{s}}x + 2D_0, 0\right) & \text{otherwise} \end{cases} \qquad \text{and} \qquad \lambda_{\mathrm{i,r}}(x,t_0) \approx \begin{cases} 0 & \text{if } x_\mathrm{f} < x \\ 1 & \text{otherwise} \end{cases}$$

where the initial shock speed D_0 and position (in the lab frame of reference) x_s were approximated from equation 2 (explained in discussion, section 5), and the fire position was approximated by $x_\mathrm{f} \approx D_0(t_0 - t_{\mathrm{ign},0})$ with $t_{\mathrm{ign},0} \sim \exp(E_\mathrm{a}(1 - D_0/D_\mathrm{CJ}))$, found by first-order integration through the induction zone (equation 1) at small times. Decay from these initial conditions agree well with theory at early times (figure 1) and an example initial profile is found in the t_0 inset of figure 2.

4 Results

The results in figure 1 show the front speed as a function of time for three different blast energies on a log-log plot. The activation energy and the induction to reaction length ratio were selected to be in the highly unstable region [15], and the blast energies were chosen to highlight three regimes of reactive blast decay. A supercritical detonation initiation is seen at the largest blast energy ($E_\mathrm{b} = 4$). Two critical regimes are shown at intermediate blast energies, with the larger case ($E_\mathrm{b} = 3$) resembling a special behaviour found in the Euler equations. Following the first pulsation, the blast enters a long sub-CJ quasi-steady period, leading to failure in the Euler case [2, 5, 7], while nearby cases ($E_\mathrm{b} = 4$ and 2.5) continue to pulsate; a slightly delayed initiation occurs in this case. The "subcritical" case is seen at the smallest blast energy. This blast decays to nearly half of the CJ speed where it remains mostly constant until two impulses (arrival of internal shocks at the front) initiate a pulsating detonation over ten times later than the supercritical case (two orders of magnitude after D_CJ was reached).

5 Discussion

To model the blast decay, start with the simplest case of an inert blast, initialized by a large ρ_b and thin x_b in the shape of a top-hat wave, with $\rho_0 = 0$ outside. The expansion fan, travelling at a speed ρ_b,

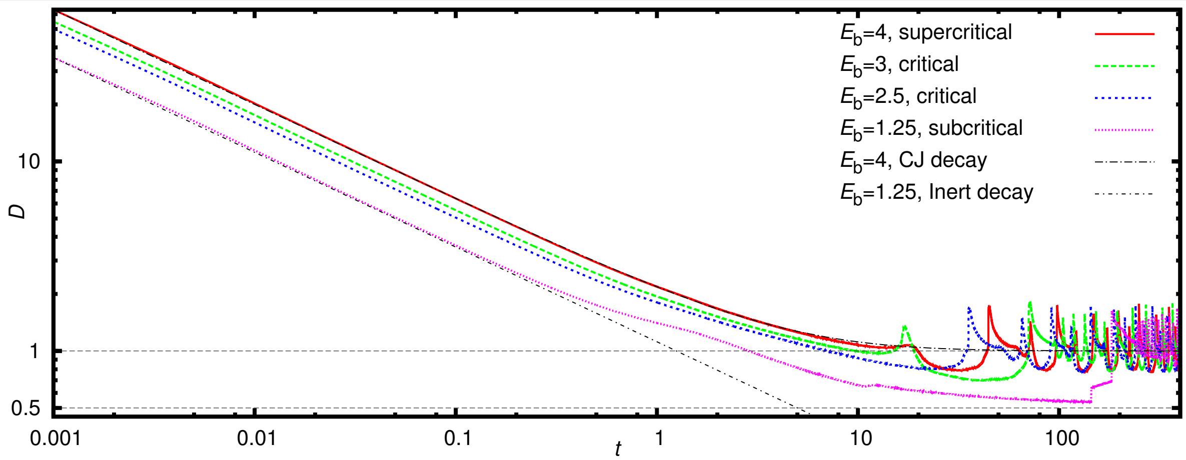

Figure 1: Numerical solutions for three different blast energies yielding supercritical and critical detonation initiations, and the subcritical case (detonation failure); inert and CJ blast decays shown for lowest blast energy case; horizontal dashed lines placed at $D_{\mathrm{CJ}} = 1$ and $D_{\mathrm{CJ}}/2$; ($E_{\mathrm{a}} = 10$, $k = 5$)

will catch up to the shock of speed $\rho_{\mathrm{b}}/2$, which will then begin decaying. Following this intersection, the shock jump condition, written as $D = \dot{x}_{\mathrm{s}} = (p_{\mathrm{vN}} - p_0)/(\rho_{\mathrm{vN}} - \rho_0)$, gives an ordinary differential equation for shock position x_{s} by attaching the expansion fan state to the post shock state, $\rho_{\mathrm{vN}} = x_{\mathrm{s}}/t$. The integration constant is found with the fan-shock intersection. The same procedure can be followed for a reaction occurring completely within the discontinuity, like a CJ wave, now with $p_{\mathrm{vN}} = \rho_{\mathrm{vN}} + Q$, and solves to

$$x_{\mathrm{s}} = \sqrt{4E_{\mathrm{b}}t + Qt^2}, \qquad D = \frac{2E_{\mathrm{b}} + Qt}{\sqrt{4E_{\mathrm{b}}t + Qt^2}}, \qquad \text{and} \qquad \dot{D} = -\frac{4E_{\mathrm{b}}^2}{(4E_{\mathrm{b}}t + Qt^2)^{\frac{3}{2}}}, \tag{2}$$

where the blast energy $4E_{\mathrm{b}} = 4(\rho_{\mathrm{b}}x_{\mathrm{b}}/2)$ comes from the integration constant. The inert case is retrieved when $Q = 0$ and the blast decays self-similarly, setting the lower bound for the blast decay. The CJ decay case, $Q = 1$, reveals the upper bound for the blast decay (instabilities aside), and is equivalent to a decay where the reaction zone is tied to the front. The two boundaries are compared to numerical simulations in figure 1 which shows the CJ decay agrees well with the supercritical case, and the inert decay describes the subcritical case until $D \sim D_{\mathrm{CJ}}/2$ (better agreement with lower E_{a}, see top inset of figure 2 for example).

Subcritical initiation can be explained by tackling the nearly constant states (shown in figure 2) in a piecewise fashion. Assume the lead shock quickly decays to $D_{\mathrm{CJ}}/2$, the state behind the fire is estimated as an expansion, the fire as an initially slow discontinuity with a jump, and a constant state to the shock (figure 2, inset $t = 10$). A series of events follows that lead to initiation: the first particle shocked at $D_{\mathrm{CJ}}/2$ reacts and the fire begins moving at $D_{\mathrm{CJ}}/2$. The moving fire creates an internal shock (inset $t = 17$) which catches the front, accelerating reaction rates and the fire. While a new internal shock from the accelerated fire reaches the front (inset $t = 25$), the first particle shocked since acceleration reacts, and the fire speed changes (inset $t = 28$). Although this type of analysis helps predict subcritical initiation time, it does not identify at what blast energies this will happen, nor the exact initial state described above.

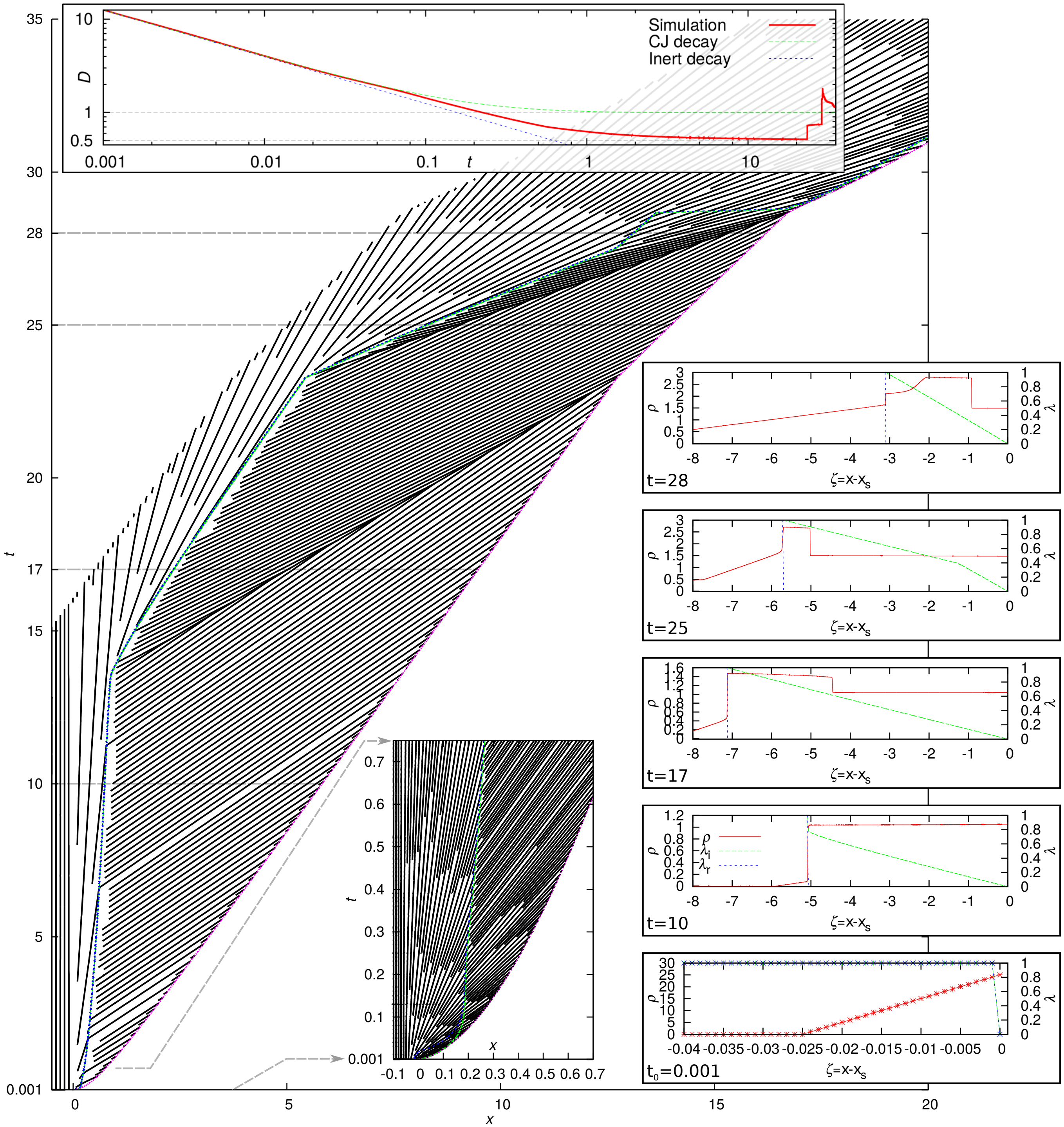

Figure 2: Characteristics diagram in the lab frame of reference ($-9 \leq x - x_{\mathrm{s}} \leq 0$) with characteristics in black, the shock front in magenta, the ends of the induction and reaction zones in green and blue, and particle paths that follow vertical lines (along which reactions take place, not shown); a magnification of early times is centred at the bottom; insets show profiles of ρ and λ on the right and blast speed at the top, see insets for their legends; ($E_{\mathrm{b}} = 5/32$, $E_{\mathrm{a}} = 5.5$, $k = 100$; ostensibly similar to the subcritical case of figure 1, with more distinct features and shorter scales)

6 Conclusion

Fickett's detonation analogue with a two-step induction-reaction model and Arrhenius sensitivity was used as an example of how simplified models may help understand direct initiation. The simplified model recreates many features of one-dimensional Arrhenius blast initiations, such as the super-, sub- and critical initiation regimes, especially a low activation energy.

References

[1] J. Lee and A. Higgins, "Comments on criteria for direct initiation of detonation," *Philos. Transactions Royal Soc. Lond. A: Math. Phys. Eng. Sci.*, vol. 357, no. 1764, pp. 3503–3521, 1999.

[2] C. A. Eckett, J. J. Quirk, and J. E. Shepherd, "The role of unsteadiness in direct initiation of gaseous detonations," *J. Fluid Mech.*, vol. 421, pp. 147–183, 2000.

[3] A. R. Kasimov and D. S. Stewart, "Theory of direct initiation of gaseous detonations and comparison with experiment," UILU-ENG 2004-6004, U. Illinois, 2004.

[4] L. He and P. Clavin, "On the direct initiation of gaseous detonations by an energy source," *J. Fluid Mech.*, vol. 277, pp. 227–248, 1994.

[5] K. Mazaheri, *Mechanism of the onset of detonation in blast initiation*. Ph.D. thesis, McGill University, 1997.

[6] M. I. Radulescu, G. J. Sharpe, and C. K. Law, "The hydrodynamic structure of detonations," in *Proc. 20th ICDERS*, (Montreal, Canada), 2005.

[7] H. D. Ng and J. H. Lee, "Direct initiation of detonation with a multi-step reaction scheme," *J. Fluid Mech.*, vol. 476, pp. 179–211, 2003.

[8] W. Fickett, "Detonation in miniature," *Am. J. Phys*, vol. 47, no. 12, pp. 1050–1059, 1979.

[9] A. Majda, "A qualitative model for dynamic combustion," *SIAM J. on Appl. Math.*, vol. 41, no. 1, pp. 70–93, 1981.

[10] W. Fickett, *Introduction to detonation theory*, vol. 5. Univ of California Press, 1985.

[11] M. I. Radulescu and J. Tang, "Nonlinear dynamics of self-sustained supersonic reaction waves: Ficketts detonation analogue," *Phys. review letters*, vol. 107, no. 16, p. 164503, 2011.

[12] L. M. Faria and A. R. Kasimov, "Qualitative modeling of the dynamics of detonations with losses," *Proc. Combust. Inst.*, 2014.

[13] A. Bellerive and M. I. Radulescu, "A nonlinear evolution equation for pulsating detonations using Fickett's model with chain branching kinetics," in *15th Int. Detonation Symp.*, (San-Francisco, USA), 2014.

[14] A. Bellerive and M. I. Radulescu, "Chaos in a Third Order Nonlinear Evolution Equation for Pulsating Detonations using Ficketts Model," in *Proc. 25th ICDERS*, (Leeds UK), 2015.

[15] S. Lau-Chadeplaine, A. Bellerive, and M. Radulescu, "Stability Characteristics of Pulsating One-Dimensional Detonations using a Simple Analogue," in *Proc. XXIV ICTAM*, (Montreal, Canada), 2016.