# Critical Dynamics of Direct Initiation of Spherical Detonations

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## 1 Introduction

Gaseous detonations can be described as supersonic combustion waves whose structure consists of an inert shock wave followed by a reactive layer [1]. The classical Chapman-Jouguet (CJ) theory predicts accurately the overall gas state behind a steady detonation front and its unique self-propagating regime considering the detonation as a discontinuity. However, the unsteady dynamics of the detonation wave are strongly sensitive to small modifications of its inner structure [2]. Hence, anticipate whether a detonation will be initiated based exclusively on the constitutive properties of the reactive mixture represents a rather difficult question. A simplified model describing the critical dynamics of direct initiation of spherical detonations in the small heat release limit is investigated here numerically. This model provides fundamental physics insights into the initiation of detonations phenomenon that may contribute to the definition of more sophisticated design specifications in the context of explosion safety.

Two different modes of initiation of a self-propagating detonation are commonly identified: direct initiation and deflagration to detonation transition (DDT). The direct initiation mode corresponds to a fast transition from a decaying blast wave into a self-sustained detonation, while in the DDT a slower transition from a deflagration to a detonation takes place. The fast mode, addressed here, is thus characterised by the absence of a predetonation deflagration.

Numerous efforts have been made to define the detonability (i.e., the potential to detonate under specific conditions) of a particular mixture. In particular, the minimum deposited energy required for direct initiation has been widely investigated. A first criterion was proposed by Zeldovich et al. [3] suggesting the time taken by the decaying blast wave to reach the CJ velocity should be larger than the reaction time. This criterion introduces the concept of a critical radius, of the order of the detonation thickness, at which the blast wave should propagate faster than the CJ velocity to initiate a detonation. However, experimental tests showed later that the critical radius is actually three orders of magnitude larger than the detonation thickness [4]. He & Clavin (1994) [5] analysed the effect of the curvature in the quasi-steady evolution of cylindrical and spherical detonations. Their study showed that flow divergence is responsible for the existence of a critical radius larger than the detonation thickness below which there is no possible solution for a self-propagating detonation. The critical radius predicted by this analysis was subsequently confirmed by Direct Numerical Simulations (DNS) [6]. Nevertheless, this model fails to explain the non-steady behaviour also observed in DNS [6–8]. The work of Liñán et al. [9] builds upon

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the quasi-steady approximation to study the external flow structure when transitioning from a strong non-reactive blast wave to a steady spherical CJ detonation. Recently, in a series of works by Clavin et al. [2, 10–12] the unsteady dynamics of detonations in the asymptotic limit of small heat release have been revisited. The asymptotic analysis including unsteadiness, curvature, and the burnt gas flow reduces the problem to a single Burgers' like equation with a reactive and a geometrical term. Numerical integration of this equation shows that this simplified model is able to reproduce to a certain extent the unsteady behaviour observed in DNS. Particularly, a deceleration of the front well below the CJ velocity and a later re-acceleration towards the self-sustained regime can be observed in the critical dynamics. Numerical results of a parametric study are presented here with special focus on the relative position of the sonic point as key driver for the critical slowdown prior to successful ignition.

## 2 Detonation model

The reactive Euler's equations in spherical geometry governing the dynamics of the inner detonation structure can be written as a set of hyperbolic equations

$$\frac{1}{\gamma p}\left[\frac{\partial}{\partial t}+(u\pm a)\frac{\partial}{\partial r}\right]p\pm\frac{1}{a}\left[\frac{\partial}{\partial t}+(u\pm a)\frac{\partial}{\partial r}\right]u=\frac{q_m}{c_pT}\frac{\omega(T,Y)}{t_r}-2\frac{u}{r}. \tag{1}$$

$$\left(\frac{\partial}{\partial t}+u\frac{\partial}{\partial r}\right)\left[\ln T-\frac{\gamma-1}{\gamma}\ln p\right]=\frac{q_m}{c_pT}\frac{\omega(T,Y)}{t_r},\qquad\left(\frac{\partial}{\partial t}+u\frac{\partial}{\partial r}\right)Y=\frac{\omega(T,Y)}{t_r}, \tag{2}$$

where $p$, $u$, $T$, and $Y$ are respectively the pressure, the radial velocity of the flow in the laboratory reference frame, the temperature, and the progress variable ($Y=0$ in the initial mixture and $Y=1$ in the burned gas), and $a$, $\gamma$, $q_m$, $t_r$, and $\omega$ are respectively the sound speed, the ratio of specific heat $\gamma\equiv c_p/c_v$, the chemical heat release per unit mass of mixture, the reaction time at the Neumann state of the planar CJ detonation and the non-dimensional heat-release rate. These equations relate the propagation of the disturbances of pressure $p$ and radial velocity $u$ to the rate of heat release $\omega/t_r$ and the divergence of the flow $2u/r$. Assuming an ideal gas model with $p=c_v(\gamma-1)\rho T$, $a^2=\gamma p/\rho$ and $\gamma=$ const., when the chemical kinetics $\omega(T,Y)$ are known, the four equations in (1) and (2) form a closed set for $p$, $u$, $T$ and $Y$.

Due to the large activation energy $\mathcal{E}$ that characterizes the combustion chemistry, the lead shock can be considered as a discontinuity in the study of the detonation structure. The boundary conditions in the initial mixture are thus given by the Rankine-Hugoniot relations with respect to the unburnt gas

$$\frac{p_N}{p_u}=1+\frac{2\gamma}{\gamma+1}(M^2-1),\qquad\frac{\rho_u}{\rho_N}=\frac{2+(\gamma-1)M^2}{(\gamma+1)M^2},\qquad\frac{u_N}{a_u}=\left(1-\frac{\rho_u}{\rho_N}\right)M, \tag{3}$$

where the subscript $u$ denotes the unburnt fresh mixture at rest and the subscript $N$ denotes the Neumann state just behind the shock. The Rankine-Hugoniot relations depend exclusively on the propagation velocity of the lead shock $\mathcal{D}$ through its Mach number $M\equiv\mathcal{D}/a_u$.

The study of the direct initiation process begins with the blast wave assumed to be produced by an intense point explosion (i.e., a sudden release of a large amount of energy concentrated at a point). The blast wave classical problem accepts a self-similar solution in the strong shock limit in which the velocity distribution evolves roughly in a linear fashion from the respective value behind the shock to the origin [1]. The initial flow field is then described by a linear profile from the Neumann state at the lead shock position to zero at the origin.

As in the detonation model of Clavin & Williams (2002) [13], the direct initiation is studied here through an asymptotic analysis in the limit of small heat release $\epsilon^2\equiv q_m/(c_pT_u)\ll 1$ coupled with the Newtonian approximation $(\gamma-1)/\epsilon\ll 1$. This distinguished limit introduces two main simplifications: the

variation of the sound speed across the detonation structure, being of order $\epsilon^2$, can be neglected to first order; and, two time scales can be identified. The propagation velocities (in the lead shock reference frame) of the acoustic downstream running wave and the entropy wave are of the order of the sound speed which is greater by a factor $1/\epsilon$ than the propagation velocity of the upstream running acoustic wave. Therefore, to first order the effects of the downstream running wave and entropy wave are considered instantaneous, and the dynamics of the inner structure is governed by the larger time scale $t_r/\epsilon$. Hence, the inner structure of the unsteady and curved detonation must be studied in terms of the non-dimensional coordinate $\xi$ attached to the moving front of the lead shock and the reduced time scale of order unity $\tau$

$$\xi \equiv \frac{r - r_f(t)}{a_u t_r}, \quad \text{and} \quad \tau \equiv \epsilon \frac{t}{t_r}. \tag{4}$$

In addition, it is convenient to introduce the dimensionless quantities of order unity in the small heat release limit as in [10]

$$\mu(\xi,\tau) \equiv \frac{1}{\epsilon}\frac{a_u - (\mathcal{D}_{o_{CJ}} - u)}{a_u}, \qquad \pi(\xi,\tau) \equiv \frac{1}{\epsilon}\frac{1}{\gamma}\ln\left(\frac{p}{p_u}\right), \qquad y(\tau) \equiv \frac{b}{\epsilon}\frac{\mathcal{D} - \mathcal{D}_{o_{CJ}}}{a_u}, \tag{5}$$

where $\mu(\xi,\tau)$, $\pi(\xi,\tau)$ and $y(\tau)$ represent respectively the normalized flow velocity, the pressure and the propagation velocity of the lead shock. A reduced form of the activation energy $b \equiv 2\epsilon(\gamma-1)\mathcal{E}/(k_B T_u)$ is also defined.

Neglecting terms smaller than $\epsilon^2$, the first order of the intrinsic dynamics of the detonation structure in the small heat release limit is governed by a single hyperbolic equation including reactive and geometric terms

$$\frac{\partial \mu}{\partial \tau} + \left(\mu - \frac{y}{b}\right)\frac{\partial \mu}{\partial \xi} = \frac{1}{2}\omega(\xi, y) - \frac{1+\mu}{\tilde{r}_f(\tau)}, \tag{6}$$

where the reduced front radius $\tilde{r}_f(\tau) \equiv \epsilon r_f/(t_r a_u)$ has been introduced. Similarly, the Neumann state condition (3) on the leading front is reduced to

$$\xi = 0: \qquad \mu = 1 + 2y(\tau)/b. \tag{7}$$

The chemical kinetics for a propagation velocity close enough to the CJ velocity $y(\tau) = \mathcal{O}(1)$ are modelled as in [5]. The unsteady distribution of the rate of heat release $\omega(\xi,\tau)$ is expressed in terms of the front propagation velocity and the steady state distribution. Accordingly, the distribution of reaction rate is governed by a scaling law depending on the reaction zone length $\xi_b$. Adopting the distribution of the steady planar CJ wave $\omega_{o_{CJ}}(\xi)$ presented in [10], the heat release distribution takes the form

$$\omega(\xi, y) = \mathrm{e}^{y(\tau)}\omega_{o_{CJ}}(\xi \mathrm{e}^{y(\tau)}), \qquad \xi < \xi_b = -\mathrm{e}^{-y} : \omega = 0. \tag{8}$$

However, this model shares the limitation of the single step Arrhenius rate law. As pointed out in [8], if the induction to reaction zone length ratio is fixed, the system will react until completion. It is required then to set a lower bound in the propagation velocity $y$ below which the reaction remains frozen

$$y \leq y_c: \qquad \omega(\xi, y) = 0. \tag{9}$$

This lower bound corresponds to the well known cross-over temperature that leads to the chemical-kinetics quenching. A value of $y_c = -b/2$ is used here considering typical values of cross-over temperature, see [11].

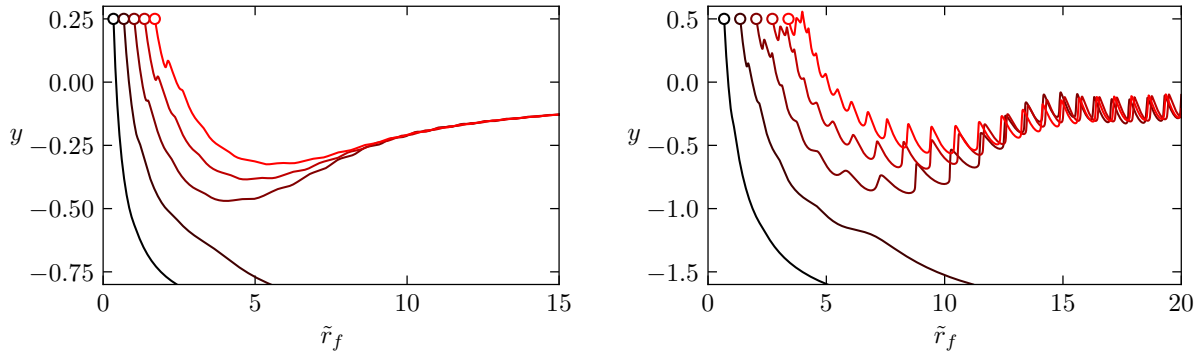


Figure 1: Trajectories 'detonation velocity $y$ vs front radius $\tilde{r}_f$' for different initial radius. Left: Stable detonation $b = 1$. Right: Weakly unstable detonation $b = 2$.

## 3 Numerical integration

In order to analyse the presented simplified model, the hyperbolic equation (6) has been integrated numerically. The numerical integration begins with a linear velocity profile as a rough approximation to the blast wave solution. Following a splitting strategy, the three terms of the hyperbolic equation are integrated successively. The convective component is evaluated using the High-Resolution Central Scheme of Kurganov & Tadmor (KT) [14]. Next, both the curvature and the reactive terms are integrated by an explicit Euler method. At the end of the integration step, a new value of the propagation velocity $y$ is computed from the solution obtained through the boundary condition (7).

The KT central scheme admits a semi-discrete formulation maintaining its high-resolution independent of $\mathcal{O}(1/\Delta t)$ [14]. Thanks to this feature, a sufficiently small time step can be chosen so that the truncation and splitting error do not degenerate the solution.

Several numerical integrations have been performed for a range of initial front radii $\tilde{r}_{fi}$, and two reduced activation energies $b$ illustrating a stable and a weakly unstable regime. For a fixed initial propagation velocity $y_i$, each initial radius $\tilde{r}_{fi}$ represents an initial deposited energy. A greater initial energy would create in a larger blast wave propagating at equal velocity, thus these two parameters are directly linked. In the chemical kinetics model investigated here, the transition from marginally stable detonations to weakly unstable detonations occurs for a value of the reduced activation energy of $b_c \approx 1.27$ [10].

## 4 Results and discussion

The different trajectories 'detonation velocity $y$ vs radius $\tilde{r}_f$' obtained are shown in Fig. 1. A stable detonation regime with $b = 1$ is presented on the left, while the evolution of a marginally unstable detonation $b = 2$ is shown on the right. The results of these stable and marginally unstable detonations are similar, except for the nonlinear oscillation superimposed on the trajectories. In both cases, successful initiation and detonation failure are observed revealing the dependence of the outcome on the initial conditions. The characteristic behaviour of the non-steady critical dynamics is also observed in both situations. After slowing down well below the CJ velocity, the detonation front re-accelerates back to the self-sustained regime. The evolution of the detonation initiation near criticality is closely related to the evolution of the sonic point $\xi_s$, where the flow velocity relative to the front equals the sound speed. In terms of the problem variables, the sonic point is located where the relation $\mu(\xi_s, \tau) = y(\tau)/b$ is satisfied. At this point, the gas flow is isolated from the damping induced by the rarefaction wave. The sonic point trajectory is shown in Fig. 2. For clarity, the stable regime has been chosen to show the

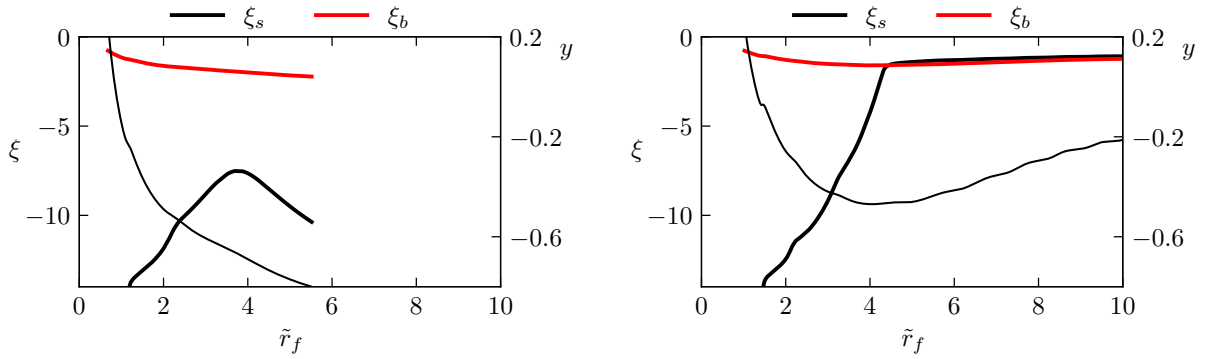


Figure 2: Sonic point $\xi_s$ and end of reaction $\xi_b$ trajectories in thick line with its corresponding 'detonation velocity $y$ vs front radius $\tilde{r}_f$' trajectory in the background for a stable detonation $b = 1$. Left: Failure of detonation initiation for $\tilde{r}_{fi} = 0.7$. Right: Successful initiation of the detonation for $\tilde{r}_{fi} = 1.0$.

sonic point $\xi_s$ and the reaction wave exit $\xi_b$ positions relative to the lead shock. The difference between figures lies in the initial front radius $\tilde{r}_{fi}$ (i.e., the initial energy). On the left, the smaller initial radius leads to a detonation failure while on the right the detonation succeeds to initiate because of the larger initial energy. The corresponding trajectory 'detonation velocity $y$ vs front radius $\tilde{r}_f$' is included in the background so that the front behaviour can be analysed in relation to the sonic point location. As the lead shock decays due to both the effect of rarefaction wave and flow divergence, the sonic point $\xi_s$ approaches the end of the reaction $\xi_b$. Once the sonic point is close enough to the exit of the reaction wave, the time delay of the detonation inner structure response to the rarefaction wave becomes relevant. Initially, the decay rate of the front is reduced and a mechanism of slowdown can be identified. As long as the chemical-kinetics quenching does not terminate the combustion, the sonic condition will be attained, i.e. the sonic point will catch the end of the reaction layer. Note that the minimum propagation velocity $y(\tau)$ for successful initiation corresponds to the sonic condition. As soon as the sonic point reaches the reaction wave, it isolates the detonation inner structure from the rarefaction wave. Then, the detonation now unaffected by the damping effect of the rarefaction wave, starts to accelerate towards the self-sustained CJ regime.

## 5 Conclusions

The asymptotic limit of small heat release reduces the mathematical description of the inner structure of a detonation to a single hyperbolic equation. This distinguished limit leverages the two-time-scale nature of the problem, which is amplified although it also characterises to a lesser extent the real detonations close to the CJ regime. The solution obtained by the numerical integration of the hyperbolic equation reveals the well known existence of a critical energy below which the direct initiation of a detonation fails. Furthermore, the usual critical dynamics, characterised by a decay well bellow the CJ velocity, followed by a re-acceleration towards the self-sustained regime, is also captured by this simple model. This behaviour is explained by the evolution of the sonic point where the velocity relative to the lead shock equals the sound speed. Initially, the propagation velocity descends below the CJ velocity while the sonic point approaches the exit of the reaction wave. As the sonic point gets closer to the end of the reaction zone, the slowdown mechanism of the wave decay is strengthened. The slowdown mechanism arises from an increase in the time delay of the response of the detonation inner structure to the trailing rarefaction wave. A minimum in the propagation velocity is observed when the sonic point reaches the inner structure of the detonation. The deceleration of the decay is followed by a re-acceleration back to the CJ regime in which the reaction zone is isolated from the rarefaction wave through the sonic

point. Hence, the sonic point remains within the detonation inner structure during the re-acceleration phase and in the self-sustained regime. The initiation process will fail if the front velocity decays bellow the chemical-kinetics quenching point before the sonic point catches the detonation structure. At small front radius, the curvature is larger and therefore the flow divergence damping is stronger, so the outcome depends ultimately on the lead front radial position at which the velocity of the overdriven detonation crosses the CJ velocity.

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