

Simple model for spherical detonation

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1 Introduction

In a recent paper [1], we have shown that a very simple model is capable of qualitatively reproducing the whole range of phenomena that one observes in one-dimensional detonations in the reactive Euler equations. The model is given by the following equation:

$$u_t + \frac{1}{2} (u^2 - uu_s)_x = f(x, u_s), \quad x \leq 0, \quad t > 0, \quad (1)$$

where $u(x, t)$ is the unknown playing the role of, say, pressure or temperature, $u_s = u(0_-, t)$ is the solution u immediately after the shock (located at $x = 0$), and f is the forcing function. The left-hand side of this equation arises from the Burgers equation by attaching the frame of reference to the shock. The forcing function on the right-hand side is taken to mimic the behavior of reaction rate in the Euler equations. In particular, strong sensitivity of f to the shock state, u_s , is its main feature. Furthermore, f is assumed to have a maximum at some distance away from the shock, $x_f = x_f(u_s)$, which depends on the shock state. If u_s is large, the maximum is near the shock, while for small u_s the maximum is far from the shock.

As shown in [1], the computation of the steady-state solutions of (1) is exactly analogous to the ZND theory, i.e. the reaction-zone structure is completely determined by solving an ordinary differential equation that is required to match the shock conditions at $x = 0$ as well as the Chapman-Jouguet conditions at the sonic point. Moreover, the model also predicts that the steady-state solutions become unstable when the source function f is sufficiently sensitive to the shock state. Numerical solutions of (1) demonstrate the existence of a Hopf bifurcation and a subsequent period-doubling cascade that leads to chaos in precise analogy to pulsating detonations in the Euler equations.

The model (1) is deceptively simple and appears to be an analog model akin to that of Fickett [2]. However, it can be shown that (1) is a consequence of the theoretical model derived by Rosales and Majda from the reactive Euler equations [3]. To establish the connection, one has to make certain simplifying assumptions to derive (1) from that theory. The most significant of these is that the rate of chemical reaction is assumed to be a function of the reaction progress variable and the shock state only. Even though this assumption results in a certain loss of generality, the resulting simplification of the

model is remarkable—it yields a single scalar partial differential equation that qualitatively retains most of the complexity of detonations in the reactive Euler equations. The equation is, however, non-local through the presence in the equation of the shock state u_s of the unknown u . The solution $u(x, t)$ at any given time t at any location x depends on the shock state, $u_s(t)$, at that time. This non-locality is a result of taking to an extreme the asymptotic idea that the waves reflecting from the shock propagate much faster than the waves moving toward the shock from the reaction zone.

A simple extension of the model by Fickett has originally been shown to reproduce the rich dynamics of unstable detonations by Radulescu and Tang [4]. These authors have also analyzed the problem of detonation ignition by a piston and elucidated the role of the ratio between the reaction-zone length and the induction-zone length in the ignition dynamics [5]. Thanks to the qualitative agreement with the detonation solutions of the full Euler equations, our model and that of [4] serve to indicate strongly that the mechanism for the complex dynamics of detonation instability might in fact be simple. Namely, for our model, that a non-linear interplay between the slow waves propagating along the forward characteristics of the Euler equations and the fast waves reflecting off the shock, may be the main reason for the instability. These latter waves are treated in (1) as propagating at an infinite speed.

In this paper, we consider an extension of (1) to model radially diverging detonations. We analyze the spherical case, but the cylindrical case is similar. Our goal is to explore the role of shock curvature in the solution and a possibility of the initiation vs failure behavior akin to that in the Euler detonations (e.g. [6]). Equation (1) written in the laboratory frame, takes the form

$$u_\tau + \left(\frac{u^2}{2}\right)_\xi = \begin{cases} f(\xi - \xi_s(\tau), u(\xi_s(\tau), \tau)), & \xi < \xi_s(\tau), \\ 0, & \xi > \xi_s(\tau), \end{cases} \quad (2)$$

where $\tau = t$, $\xi = x + \xi_s(t)$, and $\xi = \xi_s(t)$ is the shock path in the laboratory frame. The shock in this model is located at $x = 0$ with the jump condition giving the shock speed as $D = u_s/2$, when the upstream-state is assumed to be $u_a = 0$. Indeed, the Rankine-Hugoniot condition is given by $-D[u] + \frac{1}{2}[u^2] = 0$, where $[z] = z^+ - z^-$ is the jump of z across the shock. With $u^+ = u_a$ and $u^- = u_s$, we find that $D = \frac{1}{2}(u_s + u_a) = \frac{1}{2}u_s$. An extension of (1) to spherical geometry is achieved by replacing the divergence term $(u^2/2)_\xi$ in (2) by its form in spherical coordinates, $\frac{1}{\xi^2}(\xi^2 u^2/2)_\xi = (u^2/2)_\xi + u^2/\xi$. Then the shock-frame version of (1) for diverging detonations becomes

$$u_t + \frac{1}{2}(u^2 - uu_s)_x = f(x, u_s) - \frac{u^2}{x + r_s(t)}, \quad x \leq 0, \quad t > 0, \quad (3)$$

where $r_s(t)$ denotes the shock radius, which is related to the shock state as $dr_s/dt = D = u_s/2$. Thus the flow divergence acts as an energy sink competing with the forcing term f . As we show below, similarly to the Euler equations, (3) predicts quasi-steady solutions with turning points in the plane of u_s vs r_s . In addition, (3) possesses pulsating solutions, as in the planar case, however now affected by curvature.

In the remainder of this paper, we explore (3) with the purpose of demonstrating the role of curvature, $1/r_s$, in the dynamics of its solutions. We should note here that Fickett had previously considered the flow divergence in his analog model [7], and demonstrated the decrease of detonation velocity with flow divergence. However, his geometric term was quite different from ours, in addition to other differences between our models.

2 Quasi-steady solution

In this section, we look for quasi-steady solutions of (3), wherein the time derivative is assumed to be zero. Strictly speaking, the equation does not have steady-state solutions for a simple reason—as the

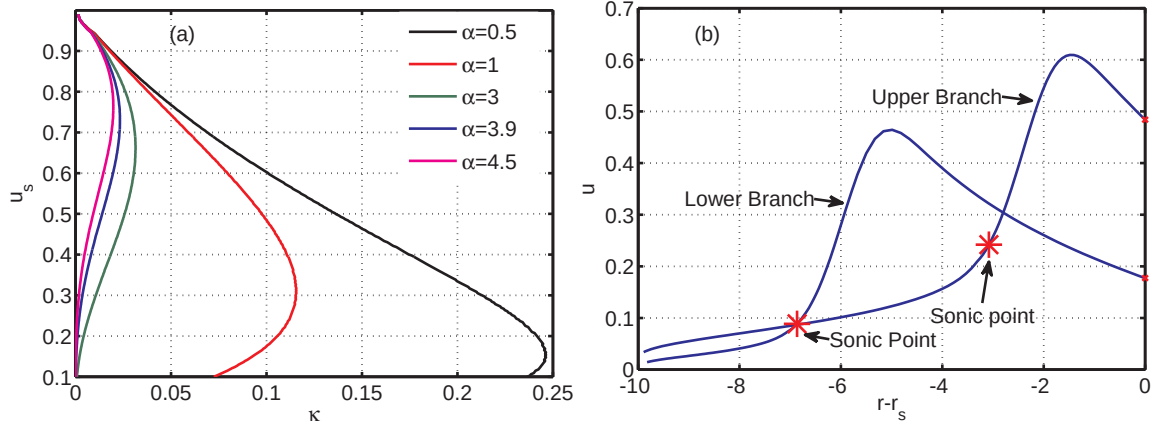


Figure 1: (a) Quasi-steady $u_s - \kappa$ curves at $\beta = 0.1$ fixed and variable α . (b) The quasi-steady solution profiles $u_0(x)$ on the top and the bottom branches of the $u_s - \kappa$ curve in (a) at $\alpha = 1$ and $\kappa = 0.1$.

shock evolves, its radius, r_s , necessarily changes in time and therefore, so does u_s and hence $u(x, t)$. Nevertheless, one can look for quasi-steady solutions by assuming that such variations of r_s in time are negligible so that at any given time, the solution structure adjusts instantaneously to the change of r_s . This asymptotic idea is precisely the main assumption in the weak-curvature theory of slowly evolving detonations (i.e. the Detonation Shock Dynamics, [8, 9]).

When u_t is dropped, (3) can be written as

$$\frac{du_0}{dx} = \frac{f(x, u_s) - \kappa u_0^2 / (1 + \kappa x)}{u_0 - u_s/2}, \quad (4)$$

where $\kappa = 1/r_s$ is the mean curvature of the shock. This equation must be solved subject to $u_0(0) = u_s$ and to some condition at $x = -r_s$, i.e. at $r = 0$. Notice that, as usual in detonation theory, there is a possibility of a Chapman-Jouguet (i.e. self-sustained) solution when there exists a sonic point, $x = x_*$, where both the numerator and the denominator of (4) vanish, i.e.

$$f(x_*, u_s) - \frac{\kappa u_*^2}{1 + \kappa x_*} = 0, \quad u_* - \frac{u_s}{2} = 0. \quad (5)$$

The solution u_* at the sonic point is obtained, for any given u_s and κ , by solving (4) from $x = 0$, where $u_0 = u_s$ to $x = x_*$, where $u_0 = u_*$. Therefore, $u_* = u_0(x_*; u_s, \kappa)$, and hence (5) is a system of two equations with three unknowns: x_* , κ , and u_s . By eliminating x_* , one obtains a relationship between u_s and κ , exactly analogous to the well-known $D - \kappa$ relation in the detonation theory [9]. The actual numerical computation of the $u_s - \kappa$ relation is a bit involved due to the saddle-point nature of the sonic point, but it can be done.

To perform specific calculations further below, we choose the same forcing function f as in [1],

$$f = \frac{a}{\sqrt{4\pi\beta}} \exp \left[-\frac{(x + u_s^{-\alpha})^2}{4\beta} \right], \quad (6)$$

except now $a = [4(1 + \operatorname{erf}(u_s^{-\alpha}/2\sqrt{\beta}))]^{-1}$ to make sure that f always integrates to the same constant. In this particular form, the model is dimensionless with u scaled so that $u_s = 1$ in the steady planar state (see [1] for details). The parameters α and β in (6) measure the sensitivity of f to the shock state

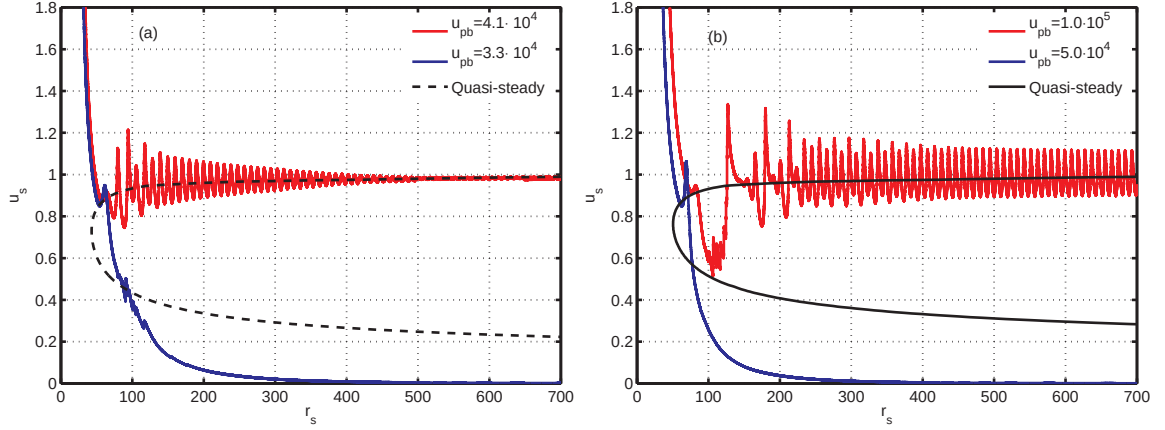


Figure 2: Initiation and failure of: (a) stable solutions at $\alpha = 3.9$ and (b) unstable solutions at $\alpha = 4.5$. In both figures $\beta = 0.1$, the computational domain length $L = 10^3$, and $N = 10^4$ grid points used.

and the width of f , respectively. They are analogous to the activation energy (α) and the ratio of the reaction-zone length to the induction-zone length (β) in the Euler equations.

In Fig. (1)(a), we show the dependence of u_s on κ for various values of α at $\beta = 0.1$. The usual turning-point behavior is seen with the turning-point curvature decreasing as α is increased. This is similar to that in Euler detonations wherein the activation energy leads to the same effects [8,9]. One important difference is that in Fig. (1)(a) there are only two branches, the lower branch tending to $u_s = 0$ and $\kappa = 0$, while in the Euler equations, there are in general three branches, the lower branch tending to $D = c_a$, the ambient sound speed, and $\kappa \rightarrow \infty$. In Fig. (1)(b), we also show the solution profiles that correspond to the $u_s - \kappa$ curves in Fig. (1)(a) at a particular value of $\kappa = 0.1$, but at two different values of u_s , one on the upper branch and one on the lower. A notable feature of these profiles is the existence of an internal maximum of u , which is absent in the planar solution at the same parameters.

3 Unsteady numerical simulations

In order to better understand the role of the curvature term in (3), we solve the problem analogous to that of the direct initiation of gaseous detonation. In the laboratory frame of reference, (3) takes the form

$$u_t + \left(\frac{u^2}{2} \right)_r = -\frac{u^2}{r} + \begin{cases} f(r - r_s(t), u(r_s(t), t)), & r < r_s(t), \\ 0, & r > r_s(t). \end{cases} \quad (7)$$

We solve this equation numerically using a fifth-order WENO algorithm and the initial conditions corresponding to a localized source of the type

$$u(x, 0) = \begin{cases} u_i, & 0 < r \leq r_i, \\ 0, & r > r_i. \end{cases}$$

Here r_i is the radius of the initial hot spot, u_i is its “temperature”. By analogy with the point-blast initiation, we keep r_i fixed at some small value and vary u_i , which is a measure of the source energy. Our findings are displayed in Fig. (2). We select two sets of parameters for α and β such that one corresponds to a stable planar solution and the other to unstable. For each case, we vary u_i to see if the detonation initiates or fails. Exactly as in the Euler detonations [10], we observe that above a certain critical value, u_{ic} , there is initiation, below—failure. Moreover, the curvature in our model also plays

a destabilizing role. As one can see in Fig. (2)(a), the detonation which is stable in the planar case, is actually pulsating in the presence of significant curvature. The pulsations are large in magnitude and irregular at first, around $r_s = 100$ to about $r_s = 150$, before settling down to regular decaying oscillations. A similar trend is seen in the unstable case shown in Fig. (2)(b) where the range of the irregular oscillations extends from about $r_s = 120$ to $r_s = 400$ before settling down to regular periodic oscillations. When the curvature has diminished significantly, the detonation dynamics is essentially that of a planar wave, hence all the phenomena observed in [1] carry over to the present study. However, the destabilizing effect of curvature clearly seen in Fig. (2) requires further analysis in order to reveal the underlying mechanisms. An additional factor that contributes to instability of the solutions is β . For planar solutions, we have shown in a separate study that smaller β lead to more unstable solutions, and we expect the same effect to preserve in the curved detonations as well.

4 Conclusions

A simple extension of [1] allows one to capture, on a qualitative level, the dynamics of radially diverging detonations. In particular, we have found that a quasi-steady solution exists which yields a relationship between the shock speed and its curvature. Analogous to the corresponding solution of the reactive Euler equations, this relationship has a turning-point behavior. We have also computed the unsteady solutions of our model equation and found that the dynamics of the point-blast initiation can be qualitatively reproduced by the model. Similarly to the Euler equations, we have found that the curvature plays a destabilizing role in the dynamics.

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