# Non-linear dynamics and route to chaos in Fickett's detonation analogue

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## 1 Introduction

Detonations waves are highly non-linear phenomena coupling the exothermicity in a medium with wave phenomena. [1] Due to the overwhelming complexity of the underlying dynamics, detonations are difficult to model analytically. In spite of these complications, it has been shown numerically that one-dimensional detonations admit universal dynamics [2] which transition to chaos via the universal Feigenbaum route of period doubling bifurcations [3] as the sensitivity of the reaction rates is increased. In fact, it can be conceived that detonations may offer an ideal physical paradigm, realizable in the laboratory, to study many other non-linear systems sharing the same universal dynamics, including hydrodynamic turbulence [ 4]. At present, because of the complexity of the governing equations and resulting dynamics, neither the one-dimensional pulsating instability nor the reason for the universality in the period-doubling detonation dynamics are currently understood.

The present study wishes to elucidate this interesting behaviour by starting with a simplified system that allows detonation-like behaviour, namely the detonation *toy-model* introduced by Fickett [ 5,6]. This toy-model is known to reproduce qualitatively many dynamic traits of real detonations, such as the wave structure, initiation transients and response to boundary losses (see [6]). Based on Burgers' equation with a source term, it also offers a much simpler mathematical framework permitting significant more insight. In the same manner that Burgers equation with random forcing offers a paradigm to study hydrodynamic turbulence [ 7], Fickett's model, which uses state-dependent deterministic forcing, can also serve to gain insight not only into detonation dynamics, but more generally into the non-linear coupling between forcing and hydrodynamic phenomena leading to instabilities.

In the following, we wish develop a reaction model bearing similarity to the real detonation structure, find the structure of its travelling wave solution and study its non-linear instability. We wish to determine if (i)the structure admits stable or oscillatory travelling wave solutions, (ii) determine the mechanism of the instability (if any) and (iii), determine if the system undergoes the universal Feigenbaum route to chaos via period-doubling bifurcations observed in the physical detonation system.

## 2 The mathematical model

The mathematical toy-model proposed by Fickett is an extension of the inviscid Burgers' equation to the reactive case, yielding:

$$\partial_t \rho + \partial_x p = 0 \tag{1}$$

$$\partial_t \lambda_r = r\left(\rho, \lambda_r\right) \tag{2}$$

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The variable $x$ has the meaning of a Lagrangian coordinate or label of a fluid particle, while $t$ represents time. [ 6] The variable $\rho$ can be ascribed the meaning of density in the reactive analogue. The flux term $p$ appearing in ( 1) has the meaning of pressure, see Ref. [6]. We choose the form proposed by Fickett:

$$p = \frac{1}{2}\left(\rho^2 + \lambda_r Q\right) \tag{3}$$

as equation of state, where $Q$ is the available energy to be released and $\lambda_r$ the fraction of the available energy remaining to be released in the medium at a given time. The second equation ( 2) provides the evolution of the energy release progress variable for each Lagrangian particle, i.e. at a fixed coordinate $x$. Note that setting $Q$ to zero, one recovers the well-studied inviscid Burgers' equation. [8]

More insight into the interplay between hydrodynamics and energy addition can be obtained by recognizing that the system of equations (1) and (2) is hyperbolic. It can be shown that the characteristic form can be written as:

$$\frac{dp}{dt} = rQ \; along \; \frac{dx}{dt} = \rho \tag{4}$$

$$\frac{d\lambda_r}{dt} = r \; along \; \frac{dx}{dt} = 0 \tag{5}$$

From 4, we deduce that the system exhibits waves propagating forward with speed $dx/dt = \rho$. The wave communicates changes in *pressure* amplitude in only the positive $x$ direction. The amplitude of the wave is not constant, but changes as a result of heat addition $Q$ at the rate $r$. Hence the model admits the physical property that waves may amplify in the presence of heat release. The second family of characteristics given by ( 5) gives the rate of energy release along a *particle path*. The physical picture emerging is thus the reactivity set out along particle paths at fixed locations $x$ modifies the strength of waves propagating forward to neighbouring particles. Through the coupling of the reaction rate (which we will ascribe below) to wave strengths, the feedback loop is closed.

Note that contrary to the physical system, which admits three sets of waves [9], the analogue only has two, as rear facing pressure waves are absent. This is the fundamental simplification over the real system which permits to gain, as will be demonstrated below, great insight into the dynamics

The system admits a coherent self-propagating travelling wave solution having the properties of a detonation [ 6]. Although the details are available in Fickett's monograph, we detail its general steady solution, as it serves as our starting point in our stability analysis. We seek a travelling wave solution to the system given by ( 1) and (2). The speed of the wave, $D$ can be found in terms of the state $(\rho, \lambda_r)$ in front of the wave (the unreacted state is $(u_0, \lambda_{r0})$) and behind the wave (the reacted state is $(\rho_2, \lambda_{r2})$). For simplicity, and without any loss of generality, we set $\rho_0 = 0$, $\lambda_{r0} = 0$ and $\lambda_{r2} = 1$ to model an irreversible exothermic reaction. We also let $\rho_2$ variable (i.e. the piston problem, see Fickett & Davis [1]). Adopting the notation $[\zeta] = \zeta_2 - \zeta_0$, the resulting wave speed can be found (see [8]:

$$D = \frac{[p]}{[\rho]} = \frac{1}{2}\frac{{\rho_2}^2 + Q}{\rho_2} \tag{6}$$

The self-sustained travelling wave solution corresponds to the case where the forward propagating characteristic trailing the wave cannot overcome the wave and modify its amplitude. The speed of this so-called limiting characteristic thus needs to be equal to the detonation speed. Denoting this special case as the Chapman-Jouguet case (by analogy to the physical system) with subscript $CJ$, we require that $\rho_2 = D = D_{CJ}$. From (6), we immediately obtain the CJ detonation speed.

$$D_{CJ} = \sqrt{Q} \tag{7}$$

Because we are dealing with an inviscid system, the detonation can be assumed to be lead by an inert shock, across which there is no energy release and the density changes discontinuously. We will denote the state behind the shock with a subscript 1 (known as the von Neumann state in the physical system). For a non-reactive shock satisfying the weak form of the inert inviscid Burgers equation, we get(e.g., from ( 6) by setting $Q = 0$)

$$\rho_1 = 2D \tag{8}$$

## 3 The steady ZND solution

The structure of the detonation wave, across which energy is deposited at a finite rate, is obtained by integrating the governing equations. The steady wave solution can be obtained by first adopting a coordinate system ($\zeta = x - D_{CJ}t - x_0, t' = t$) moving with the steady detonation. Making the formal change of variables and setting the time derivatives equal to zero in order to obtain the steady solution, we obtain:

$$\frac{d}{d\zeta}\left(\frac{1}{2}\rho^2 - D_{CJ}\rho + \frac{1}{2}\lambda_r Q\right) = 0 \tag{9}$$

$$\frac{d}{d\zeta}\left(D_{CJ}\lambda_r\right) = r \tag{10}$$

This system is integrated from the shock, with the inert shock state $\rho = \rho_1$ and $\lambda_r = 0$ as boundary condition at $\zeta = 0$, once the rate $r(\rho, \lambda_r)$ is given.

## 4 An induction-reaction model

In the present work, we propose and investigate a reaction model that captures the structure of real detonations. [ 1] Following the shock, we assume a thermally neutral induction zone, whose duration depends on the local density $\rho$ and has an Arrhenius exponential state dependence. Following the induction process, we assume an exothermic reaction that proceeds independently of the flow density. A similar model was recently investigated for the physical system by one of us [9]. The resulting generic induction-reaction model we are proposing is thus:

$$\partial_t\lambda_i = -K_i H(\lambda_i) e^{\alpha\left(\frac{\rho}{2D_{CJ}} - 1\right)} \tag{11}$$

$$\partial_t\lambda_r = K_r\left(1 - H(\lambda_i)\right)\left(1 - \lambda_r\right)^{\nu} \tag{12}$$

where $K_i$ and $K_r$ are constants controlling the times scales of the induction and reaction zones, respectively. The Heaviside function $H(x)$ controls the timing of the onset of the second exothermic reaction, which starts when the induction variable $\lambda_i$ reaches 0. Ahead of the shock, $\lambda_i = 1$ and $\lambda_r = 0$. We are also assuming that the reactions are only activated by the passage of the inert leading shock. The system to be solved is thus ( 1), (11) and (12).

## 5 The steady structure of the induction-reaction model

We now proceed to obtain the steady travelling wave solution to the system ( 1), (11) and (12). The reaction model is sufficiently simple to allow an analytical solution. Ahead of the wave in the quiescent zone, we have:

$$\zeta > 0,\ \rho = 0,\ \lambda_i = 1, \lambda_r = 0 \tag{13}$$

The induction zone terminates at

$$\zeta_i = -\frac{D_{CJ}}{K_i} \tag{14}$$

In the induction zone, we have

$$\zeta_i < \zeta < 0,\ \rho = 2D_{CJ},\ \lambda_i = 1 + \frac{K_i}{D_{CJ}}\zeta,\ \lambda_r = 0 \tag{15}$$

For a reaction order $\nu$ less than unity, the reaction layer terminates at a finite distance from the shock given by:

$$\zeta_r = \zeta_i - \frac{D_{CJ}}{K_r(1-\nu)} \tag{16}$$

In the reaction layer, we have

$$\zeta_r < \zeta < \zeta_i \tag{17}$$

$$\rho = D_{CJ}\left(1 + \left(1 + (1-\nu)\frac{K_r}{D_{CJ}}(\zeta - \zeta_i)\right)^{\frac{1}{2(1-\nu)}}\right) \tag{18}$$

$$\lambda_r = 1 - \left(1 + (1-\nu)\frac{K_r}{D_{CJ}}(\zeta - \zeta_i)\right)^{\frac{1}{1-\nu}} \tag{19}$$

## 6 Numerical technique

We now wish to investigate the non-linear stability of the travelling wave solution derived above. The system ( 1), (11) and (12) are integrated numerically starting with the steady travelling wave structure as initial condition. The numerical integration uses the fractional steps method, whereby the hydrodynamic evolution and reactive step can be performed separately. The hydrodynamic step uses Roe's approximate Riemann given in [ 10]. Owing to the simplicity of the reactive model, the reactive part of the governing equations can be solved in closed form at each time step.

## 7 Period doubling bifurcations

The system above was studied by imposing the steady wave solution as initial condition and studying its non-linear stability numerically. The results presented are for parameters, $Q = 5$, $K_i = 1$, $K_r = 2$ and $\nu = 0.5$. Below a critical value of $\alpha = 5.7$, the steady solution was found to be stable, and propagated at its constant CJ speed given by 7. Above this critical value, the travelling wave solution was unstable, and developed a stable limit-cycle. As $\alpha$ increases, the amplitude of the pulsations increase, until a period doubling bifurcation occurs at $\alpha = 6.9$. Further increases in $\alpha$ yields another bifurcation at $\alpha = 7.7$. Figure 1 shows examples of the lead shock amplitude evolution for the single mode oscillation, the twice bifurcated dynamics and a period 3 limit cycle, observed for $\alpha = 8.72$. A period 3 implies chaotic dynamics, see [2] for discussion. The results thus clearly highlight, for the first time, that the simple Fickett detonation analogue share the same universal non-linear dynamics as chemical detonations [2] and other non-linear systems.

## 8 Instability mechanism

In order to study the non-linear instability mechanism of the proposed detonation analogue, we focused our attention on the single mode instability. Figure 2 illustrates the evolution of the wave structure over approximately two oscillation periods. To visualize the dynamics, we reconstructed an (arbitrary) discrete set of pressure waves by integrating the forward characteristics given by 4 starting from arbitrary locations. We used a predictor-corrector method and interpolated on the solution obtained above. The lead shock front of the detonation corresponds to the locus where these characteristics coalesce. Behind the oscillating lead shock are the two zones of induction and reaction, represented by dotted lines. By virtue of the characteristic equation 4, the pressure waves have constant amplitude and speed everywhere except in the reaction zone, where they accelerate owing to the heat release.

By investigation of the characteristic diagram of Figure 2, the detonation phenomenon can be easily understood as the coherent wave structure formed by the amplification of forward travelling waves. These are amplified across the reaction zone and eventually reach the shock. If the reaction zone is controlled by the lead shock and the state in the induction layer, than the pressure waves continuously see the same reacting field and the self-sustained detonation phenomenon occurs.

The second interesting observation is that the pulsating detonation does not exhibit a limiting characteristic at the end of the reaction zone. Instead, characteristics enter the reaction zone from the rear, albeit at a very slow rate. In the analogue case, the characteristics entering from the rear originate from a uniform state, since waves do not

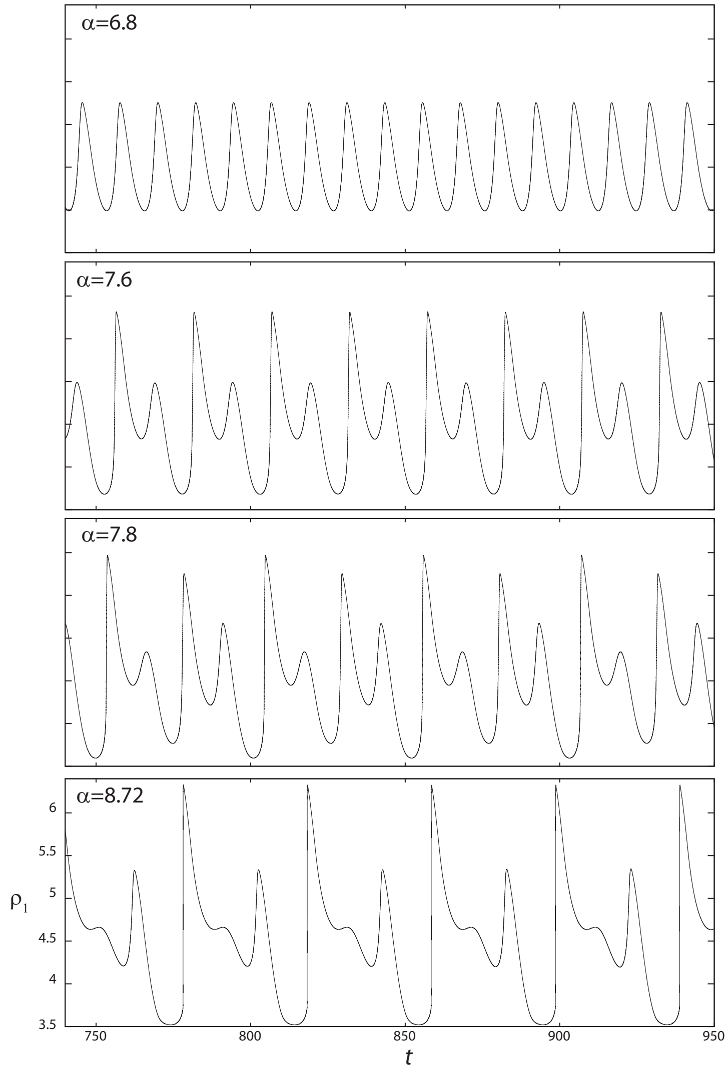


Figure 1: Shock amplitude evolution; from the top, $\alpha = 6.8$, 7.6, 7.8 and 8.72.

propagate to the rear in the analogue system. This particular feature makes the reconstruction of the instability mechanism for the detonation analogue of the present study particularly straightforward.

The instability mechanism itself can be inferred from the characteristic diagram shown in Figure 2. Because the reaction rate is state-independent, a forward facing compression wave exhibits the most amplification if it travels through the reaction zone for a long time. This can be seen by integrating 4 and taking the rate as constant, say. By inspection of Figure 2, the amplification part of the cycle occurs when the reaction zone commences at an earlier time and the induction delay is short, as to permit the pressure waves to reside in the reaction zone for longer times. In our system, this occurs because of the induction time dependence on shock strength. With increasing shock strength, the induction delay is shorter, the reaction zone commences earlier, the pressure waves passing through the reaction zone amplify more, arrive at the leading shock stronger and hence amplify the leading shock. Note that the same mechanism also occurs in the real system [9] where compression waves in phase with the energy release amplify more by the so-called SWACER mechanism. The deceleration, restoring, mechanism relies on the same principle: waves coming from the back and passing quickly across the reaction zone get less amplification and contribute to decelerate the leading shock. It thus appears that these two competing mechanisms are at the heart of the instability. In fact, they can be viewed as a continuous extension to Toongs' original model in a square wave detonation. [11] In McVey and Toong's model, a sudden shortening of the induction zone provides a forward

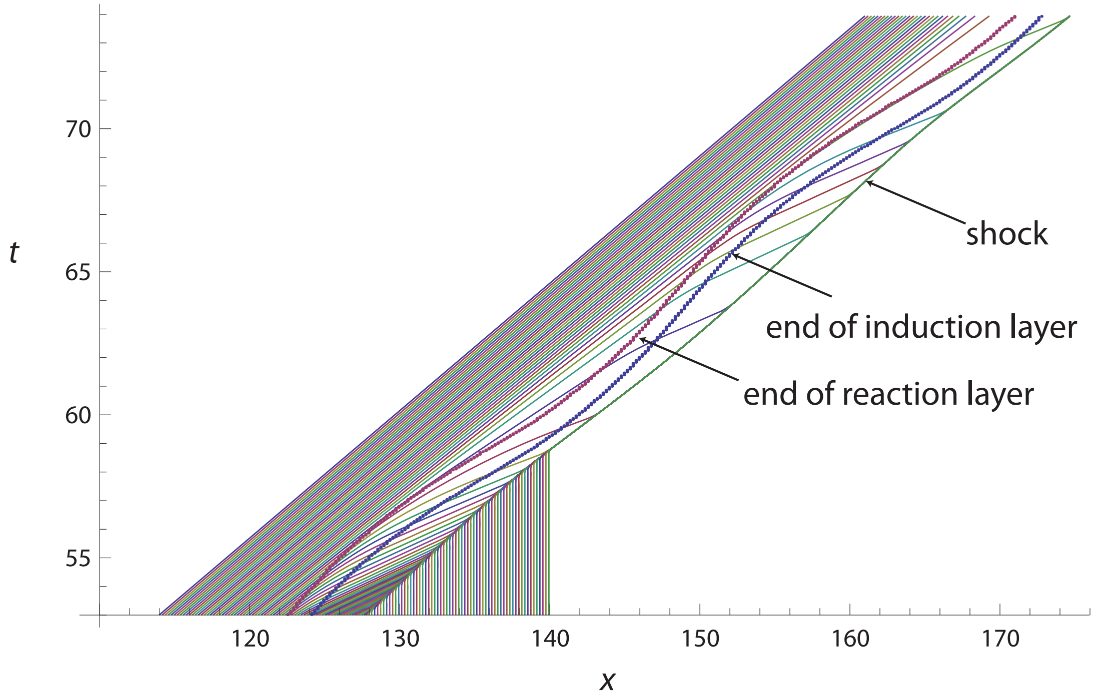


Figure 2: Space time diagram illustrating the pressure waves in the reaction zone of a pulsating detonation.

facing shock, followed by a forward facing expansion wave shortly after, once the reactions are terminated along the particle path.

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