# Chaos in a Third Order Nonlinear Evolution Equation for Pulsating Detonations using Fickett's Model

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## 1 Introduction

Detonations are self-sustained supersonic waves consisting of a shock front that is driven by a volumetric expansion induced by chemical reactions of the shocked material. The minimum sustainable steady detonation speed is known as the Chapman-Jouguet (CJ) detonation velocity, where the detonation velocity is the speed at which the fully reacted zone flow is exactly sonic relative to the lead shock. In practice, detonations are rarely stable and have two main instability modes: one-dimensional pulsating or multi-dimensional cellular. Stability characteristics have been correlated with the natural tendency of a reactive mixture to detonate [1]. Additionally, unstable detonations have wider limits [1, 2] when compared to stable ones. Asymptotic methods have been used on the Reactive Euler Equations to achieve analytical solutions by many researchers, to predict such stability characteristics.

The typical strategy in asymptotic modeling is formulated using a combination of the following: the limit of large activation energy [3, 4], the Newtonian limit [5], overdriven detonation limit [6], and/or the limit of weak heat release [7, 8, 9]. Nevertheless, such methods become very complex and limit high order analysis of the Reactive Euler Equations due to strong nonlinearities. Alternatively, direct numerical simulation captures the nonlinearities, but recovering the explanation why some detonation are more unstable than others is difficult.

For instance, numerical simulations on the Reactive Euler Equations have shown that increased instability, caused by increasing the activation energy, leads to higher modes of oscillation [10]. These higher mode oscillations arise from period doubling bifurcations and lead to chaos, but the nonlinear mechanisms remain unknown. Similar results were found using simple detonation analogues [11, 12, 13].

Fickett, and Majda introduced simple detonation analogues as a variation of Burgers' equation [14] by adding an energy release term. Fickett's model [15, 16] has two families of waves, forward traveling pressure waves and energy release along the particle path. The Majda model [17] has forward traveling waves and infinitely fast backward traveling waves, i.e., instantaneous, and also demonstrated the route to chaos [12, 13].

Fickett's model proved useful in numerical simulation and asymptotic modeling of piston initiated detonations [18]. It was also useful in stability analysis using asymptotic modeling [19], where a second order evolution equation was derived. The second order equation was used to find an analytical stability

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boundary, where at small ratios of induction to reaction time it was found to be the non dimensional $\chi$ parameter, the product of induction to reaction time and the activation energy $\chi = (t_{ind}/t_{reac})E_a = 4$, and at large ratios of induction to reaction times it was found to be $E_a = 4$.

The present work focuses on asymptotic modeling by extending the work done by Short [4] on the Reactive Euler Equations to higher order on Fickett's model. A two-step, induction-reaction, reaction model is used, which was studied in detail by Short & Sharpe [20], Ng et al. [21], and Leung, Radulescu & Sharpe [22] for the Reactive Euler Equations, and by Radulescu and Tang [11, 18] for Fickett's model. The simplicity of Fickett's model coupled with the two-step reaction model can serve to study the higher mode oscillations without the complexity of the strong nonlinearities of the Reactive Euler Equations, while still reproducing the complex detonation dynamics [11]. In addition, $O(\epsilon^3)$ analysis, as done in this paper with Fickett's model, are nearly impossible on the Reactive Euler Equations, due to it's complexity. Analytical solutions to the pulsating detonations in Fickett's model are sought using asymptotic expansions at the limit of high activation energy.

The paper is organized as follows. First, the model is presented and an oscillator equation is derived for the lead shock perturbation speed, which takes the form of a third order nonlinear ODE. The dynamics predicted by the oscillator are then discussed.

## 2 Model

The detonation wave is modeled with Fickett's equations [16], an analogue to the compressible Reactive Euler Equations. The model is of the same form as the inviscid Burgers' Equation [14], $u_t + uu_x = 0$, with an added energy release term. Fickett's model in the shock attached frame of reference is given by two equations, the conservation equation

$$\frac{\partial}{\partial \tilde{n}}\left(\tilde{\rho}^2 - \tilde{D}\tilde{\rho} + \frac{1}{2}\lambda_r Q\right) = -\frac{\partial \tilde{\rho}}{\partial t}, \tag{1}$$

and the reaction rate equation

$$\frac{\partial \lambda_{(i,r)}}{\partial \tilde{n}} = \frac{1}{\tilde{D}}\left[\frac{\partial \lambda_{(i,r)}}{\partial t} - \tilde{r}_{(i,r)}\right], \tag{2}$$

where $\tilde{n}$ is the space coordinate in the shock attached frame, $\tilde{\rho}$ is analogous to density, $D$ is the shock speed, $r_r$ is the reaction rate, $r_i$ is the induction rate, $\lambda_i$ is the induction progress variable, $\lambda_r$ is the reaction progress variable, and $Q$ is the heat release parameter. The modeled detonation structure is assumed to have a two-step reaction. The first step is thermally neutral, i.e., no heat release. The second step is exothermic and independent of the thermodynamic state, i.e., independent of $\tilde{\rho}$ or $\tilde{D}$. The chain-initiation dynamics in the induction zone are controlled by a Detonation velocity-sensitive Arrhenius reaction rate,

$$\tilde{r}_i = -K_i \exp\left(E_a\left(\frac{\tilde{D}}{2D_{cj}} - 1\right)\right), \tag{3}$$

where $D_{cj}$ is the CJ detonation velocity, $K_i$ is the constant of reaction, and $E_a$ is the activation energy. $K_i$ controls the induction zone length, and $E_a$ controls the sensitivity to changes in detonation velocity, $\tilde{D}$. The progress variable $\lambda_i$ is equal to 1 at the shock front and 0 at the end of the induction zone, where the heat release is then triggered. The energy release rate equation is of the form

$$\tilde{r}_r = K_r(1-\lambda_r)^{\nu}, \tag{4}$$

where $K_r$ is the reaction constant, and $\nu$ is the reaction order. The reaction order is assumed to be such that $1/2 \le \nu < 1$. A reaction order of non-unity is used to approximate several steps of chain-branching and chain termination that is typically found. $\lambda_r = 1$ signals the rear equilibrium or sonic point of the detonation wave.

## 3 Evolution equation

The evolution equation is derived assuming a high activation energy, $E_a = \epsilon^{-1}$, $\epsilon \ll 1$, a longer reaction to induction time, $K = K_r K_i^{-1} \ll 1$, and a slow pulsating evolution time, $\tau = \epsilon t$, where t is scaled to the induction delay time. The steady detonation wave, traveling at the CJ velocity, is perturbed by a small velocity, such that the space coordinate in the shock attached frame is now written

$$\tilde{n} = \tilde{x} - D_{cj} t + \tilde{h}, \tag{5}$$

where $\tilde{h}$ is the position of the perturbed shock relative to the steady CJ detonation wave. The scaled governing Eqs. (1) and (2), respectively, are then written

$$\frac{\partial}{\partial n}\left(\rho^2 - \left(1 + \epsilon h_\tau\right)\rho + \frac{\lambda_r}{4}\right) = -\epsilon \frac{\partial \rho}{\partial \tau}, \text{ and} \tag{6}$$

$$\frac{\partial}{\partial n}\lambda_{(i,r)} = \frac{1}{1 + \epsilon h_\tau}\left[\epsilon \frac{\partial \lambda_{(i,r)}}{\partial \tau} - r_{(i,r)}\right]. \tag{7}$$

Removing the tildes ($\tilde{}$) denotes scaled variables with respect to the induction zone values in the steady detonation wave solution, see [19] for the full problem framework. Similarly, the scaled reaction rates for the induction and reaction zone are

$$r_i = -\exp\left(\frac{1}{\epsilon}(D - 1)\right), \text{ and} \tag{8}$$

$$r_r = K(1 - \lambda_r)^\nu, \tag{9}$$

respectively, where $r_i$ is scaled to the induction time, and the detonation velocity is $D = 1 + \epsilon h_\tau$. Following perturbation theory, the variables are assumed to have solutions of the form

$$\rho = \rho^{(0)} + \epsilon\rho^{(1)} + \epsilon^2\rho^{(2)} + \epsilon^3\rho^{(3)} + O(\epsilon^4) + ..., \tag{10}$$

$$\lambda_r = \lambda_r^{(0)} + \epsilon\lambda_r^{(1)} + \epsilon^2\lambda_r^{(2)} + O(\epsilon^3) + ..., \tag{11}$$

where $\rho^{(0)}$ and $\lambda^{(0)}$ are the steady solutions [23]. The expansion Eqs. (10) and (11) are substituted into Eqs. (6-9), which are then integrated across the detonation wave at $O(\epsilon)$, $O(\epsilon^2)$, and $O(\epsilon^3)$. At each order, a singular solution arises at the sonic point ($\lambda_r = 1$). As a result, a condition is needed to satisfy the governing Eq. (6) at each order. Combining these conditions up to $O(\epsilon^3)$ result in the third order in time nonlinear evolution equation in the shock velocity perturbation:

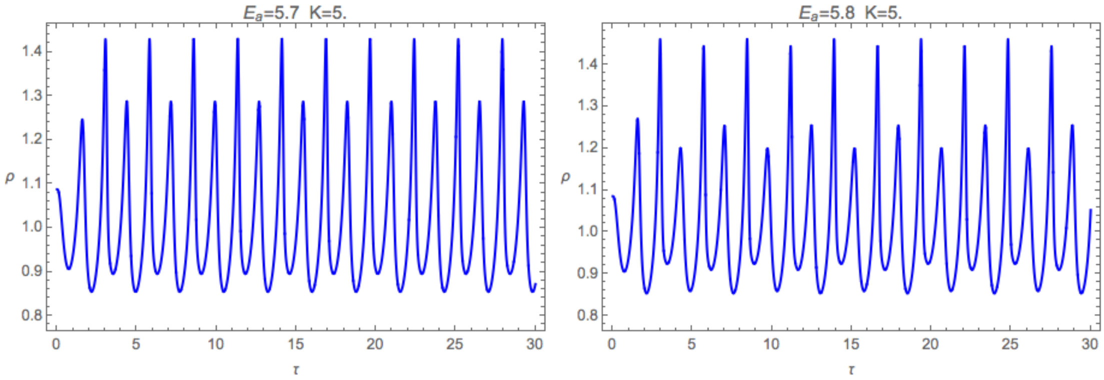
$$\begin{aligned} 3h_\tau - F_\tau + \epsilon\left(\frac{7 - 4\nu}{4K(\nu - 1)(2\nu - 3)}(h_{\tau\tau} + F_{\tau\tau}) - h_{\tau\tau}F - h_\tau F_\tau\right) \\ + \epsilon^2\left\{\left(\frac{9 - 4\nu}{2K(-1 + \nu)(-3 + 2\nu)(6 - 8\nu)} - \frac{1}{4K(-1 + \nu)(-3 + 4\nu)}\right)(F_{\tau\tau\tau} + h_{\tau\tau\tau})\right\} = 0, \end{aligned} \tag{12}$$

where $F$ is the length of the induction zone:

$$F = F(\tau) = -\exp(-h_\tau), \tag{13}$$

which is found by integrating the induction rate Eq. (8). The first two terms in Eq. (12) originate from the integration of $O(\epsilon)$, the group of terms multiplied by $\epsilon$ originate from the integration of $O(\epsilon^2)$, derivation up to this point can be found in [19]. Extending the work to higher order results in the group of terms multiplied by $\epsilon^2$, which originate from the integration of $O(\epsilon^3)$. Secular terms have appeared at $O(\epsilon^3)$ using the current expansion. They include nonlinear terms in $F_{\tau\tau\tau}$ (only the leading term $h_{\tau(4)}\exp(h_\tau)$ is used), the $\lambda^{(3)}$ solution, $(h_\tau + F_\tau)^3$, and $(F_\tau + h_\tau)(F_{\tau\tau} + h_{\tau\tau})$. These were omitted in the following analysis.

The $O(\epsilon^3)$ integration results in a third order term ($h_{\tau(4)}$) which arises from $F_{\tau\tau\tau}$ in Eq. (12), thus allowing the possibility of period doubling bifurcations.




(a) (b)

Figure 1: Shock front density history for (a) a period two solution at $K = 5$ and $E_a = 5.7$, and (b) a period four solution at $K = 5$ and $E_a = 5.8$.

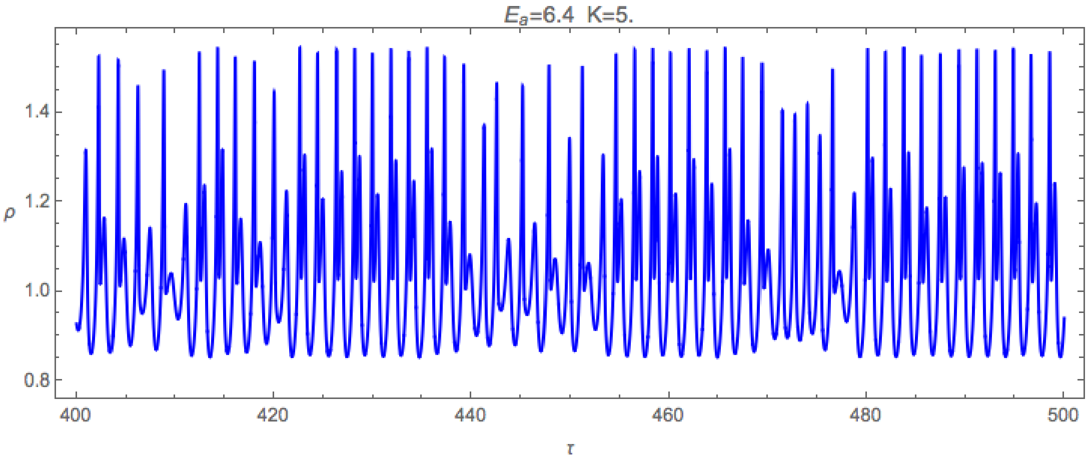



Figure 2: Shock front density history, $\rho = 1 + (1/E_a)h(\tau)$, for a chaotic solution after $\tau = 400$, no periodicity was observed.

## 4 Results

The third order evolution Eq. (12) was solved using fourth order Runge-Kutta algorithms with initial conditions close to the steady solution to simulate small perturbations. The parameters used are $K = 5$, $\nu = 1/2$, and $E_a$ is varied. A period two solution and a period four solutions is shown in Fig. 1(a) and (b). Their respective periods are $\tau = 2.67$ and $\tau = 5.45$, hence the period doubling bifurcation. The period doubling continues and cascades to chaos, as shown in Fig. 2 for higher $E_a$, where no periodicity was found. A bifurcation diagram is shown in Fig. 3, where the density maxima and minima of the shock front is plotted. In addition, a period three solution was found near the point $E_a = 6$, thus confirming the chaotic solution. The similarities of the bifurcation diagram (Fig. 3) compared to the Reactive Euler case [10] are strikingly similar, despite the simple form of Fickett's model.

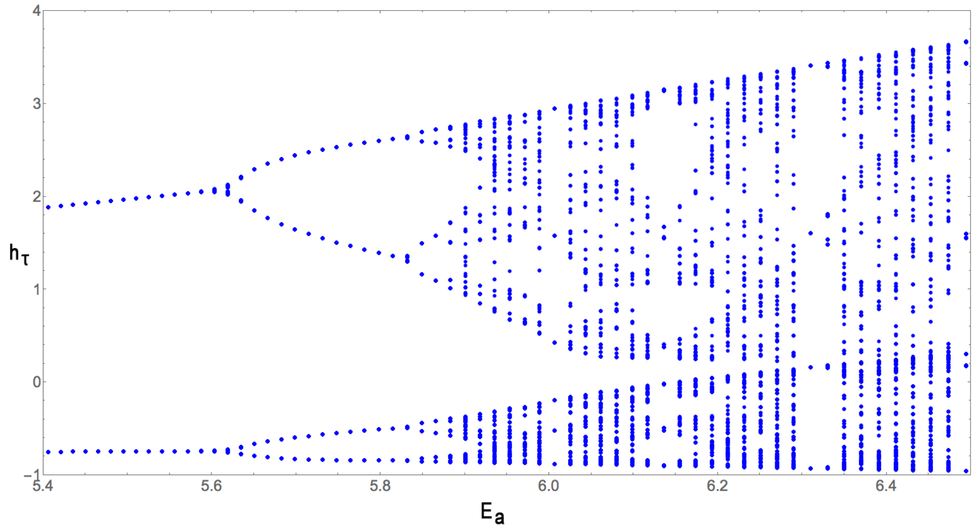



Figure 3: Bifurcation diagram for $K = 5$ showing the relative velocity maxima (top branch) and minima (bottom branch). Note, density is given by $\rho = 1 + \epsilon h_\tau$. The Hopf bifurcation was omitted, it occurs at $E_a = 4.2,\ h_\tau = 1$.

## 5 Concluding Remarks

Perturbation theory was applied on Fickett's model to $O(\epsilon^3)$ of the inverse activation energy, $\epsilon = 1/E_a$, resulting in a third order in time nonlinear evolution equation in the shock velocity perturbation. The evolution equation undergoes a Hopf bifurcation, followed by a period doubling cascade to chaos. Terms were omitted at $O(\epsilon^3)$ due to the singular nature of the expansion at this order. However, the results agree with numerical simulation on the same model as well as having many similarities with the Reactive Euler Case.

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