Numerical Investigation of One-dimensional Pulsating Detonations Using Fickett's Detonation Analogue with Chain-Branching Kinetics

Aliou Sow * and Matei Radulescu
University of Ottawa
Ottawa, Canada/Ontario

1 Introduction

Gaseous detonations seldom have a laminar steady structure. The majority of detonation waves exhibit three-dimensional unstable time-dependent cellular structures with inherent instabilities [1, 2]. Considering these instabilities is key to determine the dynamic parameters such as initiation energy, critical tube diameter, and detonation limits. While instabilities manifest themselves as nonlinear longitudinal pulsations in one-dimension, in higher dimensions transverse instabilities are also present. The origin and the role of these instabilities, however, are still not well understood.

In the past, analytical or numerical approaches have been used to study the detonation stability [3–8]. The analytical approach deals mainly with weak disturbances and mostly consider one-step chemistry laws. Although very useful to determine the neutral stability region, the analytical method can not accurately predict the long time dynamics. In contrast, the numerical approach gives the neutral stability region and the long time behaviour of the system. Furthermore, the numerical modeling is often based on one-dimensional reactive Euler equations with a one-step Arrhenius reaction rate law. As the controlling parameter - the activation energy - is moderately increased, the detonation goes from linearly stable modes to linearly unstable period-one oscillations. Further increasing the activation energy leads to chaos through period-doubling in accordance with Feigenbaum's cascade bifurcation [7]. The limitation in these simulations is related to the one-step chemistry model used. For instance, hydrogen diluted mixtures can not be reproduced using a single-step chemistry. In deed, in a single-step model the thermally neutral induction zone and the reaction length can not be controlled independently. To overcome this difficulty, two-steps chain-branching models have been utilized [6, 9]. Detonations with a long exothermic reaction length are stable or weakly unstable while detonations with a short exothermic reaction length are unstable or highly unstable. It was proposed that the stability is better described by the product of the activation energy and induction to reaction length ratio [10]. At present, however, a detailed description of the detonation dynamics for short and long reaction time scales is yet to be carried out.

Our aim here is to investigate, away from the neutral stability boundary, the spatiotemporal nonlinear dynamics of detonations in a wide range of reaction time scales. To this end, using a Fickett's detonation analogue, we conducted a detailed parametric study with close to four thousand simulations.

Correspondence to: asow2@uottawa.ca

2 Governing Equations and Numerical Methods

The Fickett's mathematical model for detonations is used with a generic induction-reaction model proposed in [9] to model the chemistry. The governing equations written in the shock-attached frame are:

$$\begin{aligned}\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}(p-D\rho) &= 0\\ \frac{\partial \lambda_i}{\partial t}+\frac{\partial}{\partial x}(-D\lambda_i) &= -k_i H(\lambda_i) e^{[\alpha(\rho/2D_{\mathrm{CJ}}-1)]}\\ \frac{\partial \lambda_r}{\partial t}+\frac{\partial}{\partial x}(-D\lambda_r) &= k_r[1-H(\lambda_i)](1-\lambda_r)^{0.5}\\ \frac{dD}{dt} &= \frac{d\rho}{dt}\left(\frac{d\rho}{dD}\right)^{-1}\end{aligned}$$

Where D is the detonation speed. $D_{\mathrm{CJ}}=\sqrt{q}$ is the Chapman-Jouguet speed. α is the activation energy. $p=\frac{1}{2}(\rho^2+\lambda_r q)$ has the meaning of pressure; ρ has a meaning of density. q is the heat release and α the activation energy. λ_i and λ_r are the induction and progress variables. k_i and k_r are constants controlling the induction and reaction time scales. Note that all variables are dimensionless, see reference [11] for more details.

A shock-fitting numerical algorithm using a WENO5M scheme [7, 12, 13] for spatial integration and a third order Runge–Kutta scheme for time advancement is employed. To adequately capture the detonation dynamics at least 256 grid points per unit length are used. The maximum numerical resolution used is 1024 grid points per unit length. The steady state solution of the governing equations is used as initial solution for the transient computations.

3 Results

For all computations in this paper, q and k_i are set to 5 and 1, respectively. By sampling over different α and k_r the neutral stability boundary is obtained numerically as shown in Fig. 1. In the limit of slow reactions, $k_r << 1$, the stability is controlled by αk_r. In the limit of fast reactions, $k_r >> 1$, the reaction time scale becomes very small. Changes in k_r will not modify the detonation structure. The stability is uniquely controlled by α. This result was first reported by Tang [11].

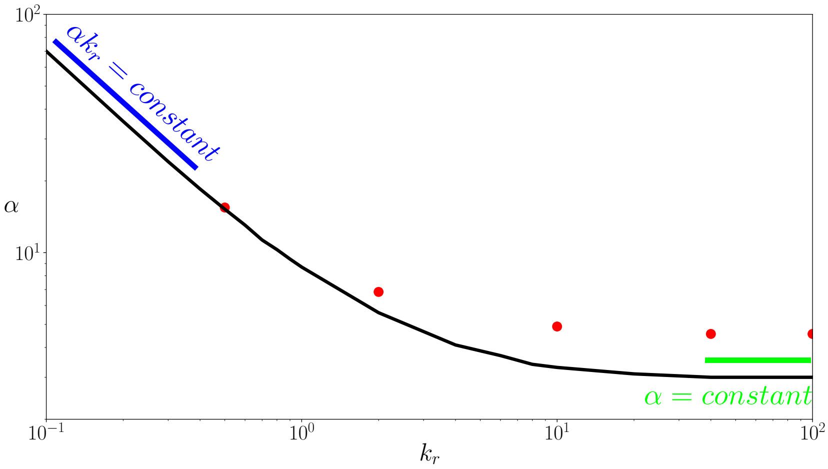

Figure 1: Neutral stability region (black line) and first bifurcation point with period-2 oscillations.

To analyze the detonation dynamic away from the neutral stability, the period-2 bifurcation locations are presented in Fig. 1. In the limit of short reaction times the period-2 oscillation bifurcation location becomes insensitive to k_r. As k_r is reduced gradually, the period-2 bifurcation locations lean towards the neutral stability curve. In the limit of long reaction times, for instance $k_r = 0.5$, the period-2 bifurcation location is very close to the neutral stability boundary. To further investigate the stability, we constructed detailed bifurcation diagrams for $k_r = 0.5$, $k_r = 2$, and $k_r = 100$. The results are depicted in Figs. 2-4. At $k_r = 0.5$, for $\alpha < 15.335$ the system is linearly stable. The period-doubling bifurcations

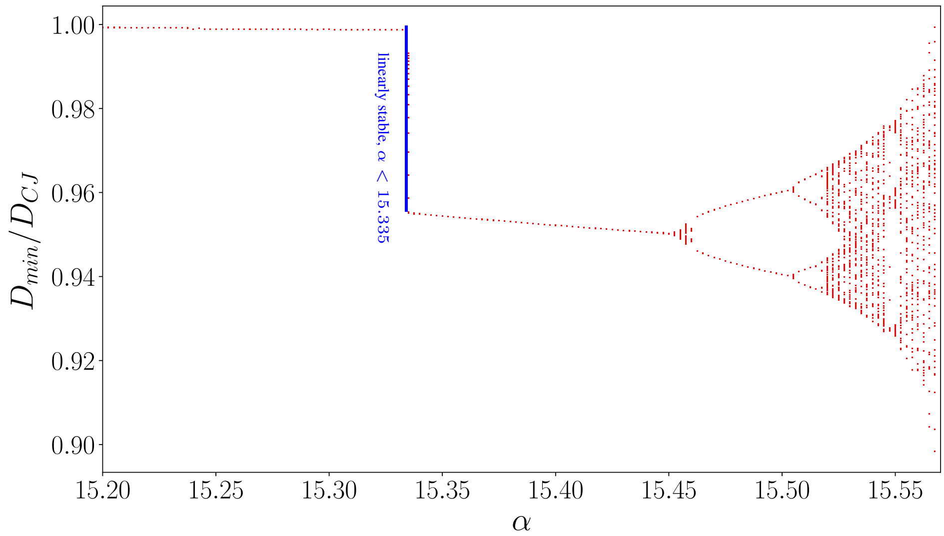

Figure 2: Bifurcation diagram for $k_r = 0.5$. A sampling of 154 activation energies corresponding to $\Delta\alpha = 0.0025$.

are clearly seen for $\alpha > 15.335$. We can also notice the apparent chaotic behaviour. Similar observations was found previously [6, 7]. Notice that the neutral boundary is at a relatively high α (15.22) and the nonlinear dynamics occurs within a small window of α.

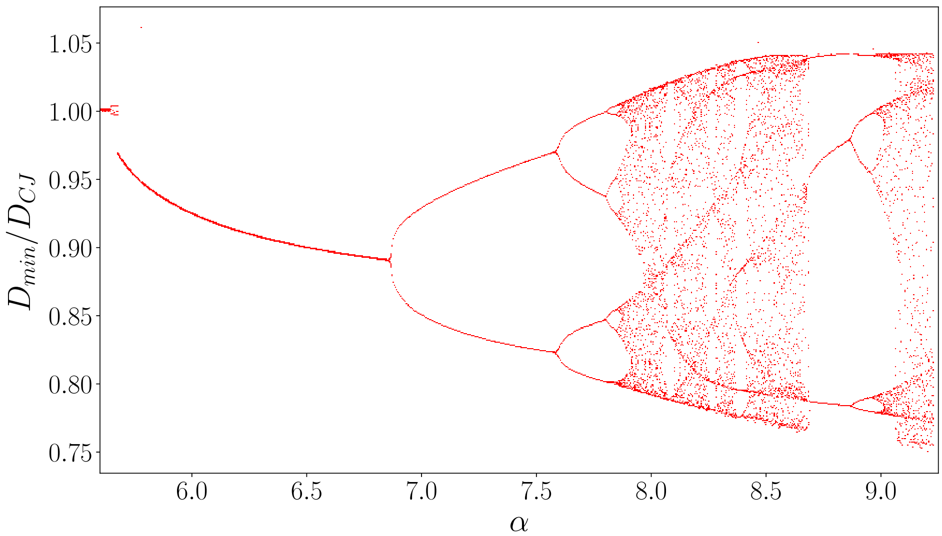

Figure 3: Bifurcation diagram for $k_r = 2$. A sampling of 2900 activation energies corresponding to $\Delta\alpha = 0.00125$.

At $k_r = 2$, a sampling of 2900 activation energies is considered allowing to have a better qualitative agreement with the logistic map, see Fig. 3. Compared to the case $k_r = 0.5$, the nonlinear dynamics take place in wider window of activation energies. This can be seen by comparing the bifurcation points at period-4 oscillations.

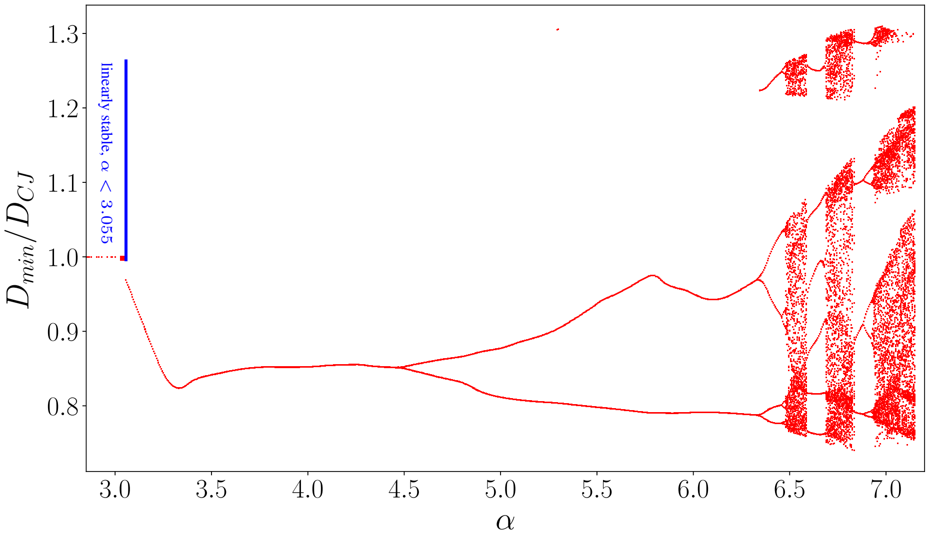

Figure 4: Bifurcation diagram for $k_r = 100$. A sampling of 861 activation energies corresponding to $\Delta\alpha = 0.005$.

At $k_r = 100$ the period-doubling classical route to chaos is not observed. We have period-1, period-2, period-5 oscillations. Period-4 and period-8 oscillations are not activated in the initial period-doubling cascade. The question naturally arrises: why such differences in the route to chaos?

Figure 5 shows the detonation time histories for $k_r = 100$ at different activation energies. The detonation is quenched for a short time before the appearance of a period-2 oscillation, see Fig. 5-b and c. At this stage the shock and the reaction zone are decoupled and the inert shock propagates at a constant speed. The measured reignition times for $\alpha = 4.75$ and $\alpha = 6$ are $t = 3.661$ and $t = 5.552$, respectively. From the equation of the induction variable the theoretical ignition time can be obtained. It is given by $t_{ignition} = 1/\exp[\alpha(1/\sqrt{2} - 1)]$. The analytical ignition times are $t = 4.019$ and $t = 5.797$ for $\alpha = 4.75$ and $\alpha = 6$, respectively. The numerical and analytical ignition times are in good agreement. Besides, galloping detonations are observed after the detonation reignition. The difference on the path to chaos is a consequence of the process of failure and reignition.

4 Discussions

For long reaction time scales, $k_r < 0.5$, the detonation is linearly stable for a wide range of activation energies. From the neutral stability boundary, a marginal increase in the activation energy causes the detonation to quench. For instance, at $k_r = 0.2$, the neutral stability boundary is at $\alpha = 35.55$, the detonation quenches at $\alpha = 35.8$. From the neutral boundary to the point at which quenching occurs, the detonation is either stable or weekly unstable. The instabilities keep growing for very long times before the detonation fails, see Fig. 6. For such scenario period-doubling bifurcations is not observed in this study.

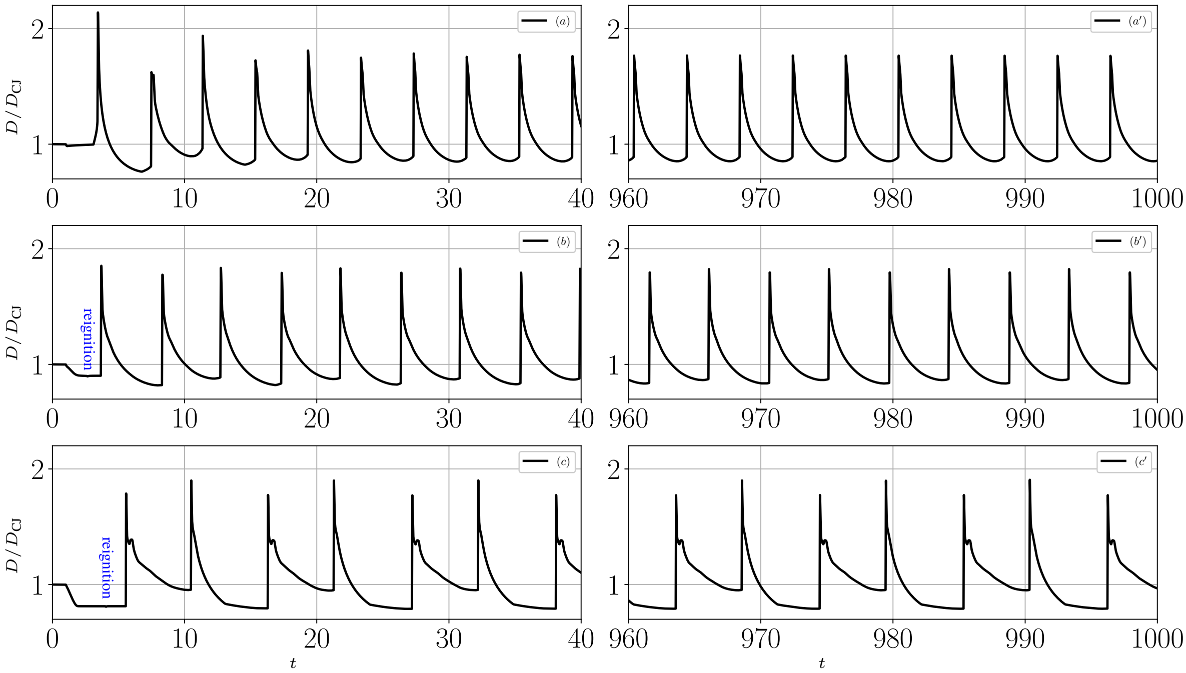

Figure 5: Time history of detonation velocity for $k_r = 100$. a) and a') $\alpha = 4$; b) and b') $\alpha = 4.75$; c) and c') $\alpha = 6$.

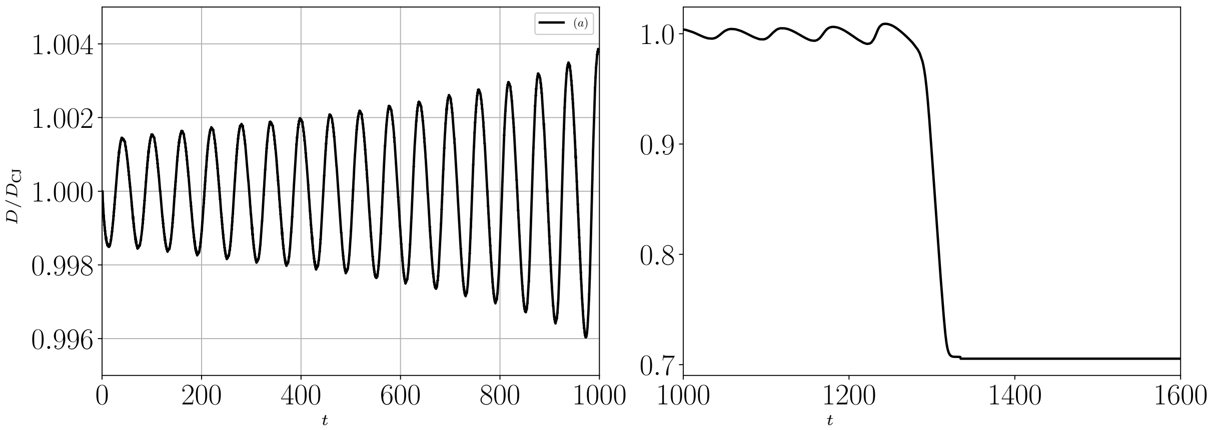

Figure 6: Time history of detonation velocity for $k_r = 0.2$ and $\alpha = 35.8$.a) Initial times; b) Late times.

For intermediate reaction time scales the traditional period-doubling cascade to chaos scenario is observed. On the other hand, for short reaction time scales, $k_r > 39.9$, the route to chaos is different. The detonation fails prior to the establishment of period-2 oscillations. It is only after the reignition of the detonation that period-2 oscillations are observed. For these short reaction time scales period-4 and period-8 oscillations are skipped in the route to chaos. Since most gaseous detonations are characterized by short reaction times, more efforts should be dedicated into the region of high k_r. We are conducting additional parametric studies to better characterize the detonation dynamics for vanishing reaction times. The challenges in these studies are related to the high numerical resolution needed to accurately capture the square wave reactions.

References

[1] J. Lee (2008). The Detonation Phenomenon. Cambridge University Press, 2008.

[2] F. Zhang (2009). Shock Wave Science and Technology Reference Library. Springer, vol 6, Detonation dynamics.

[3] M. Short (2001). A nonlinear evolution equation for pulsating Chapman-Jouguet detonations with chain-branching kinetics. J. Fluid Mech., vol. 430, pp. 381-400.

[4] G.J. Sharpe, Linear stability of idealized detonations(1967). Proc. of the Royal Society of London Series A – Mathematical Physical and Engineering Sciences, vol 453 (1997) 2603–2625.

[5] H.D. Ng , A.J. Higgins , C.B. Kiyanda , M.I. Radulescu , J.H.S. Lee , K.R. Bates , N. Nikiforakis (2005). Nonlinear dynamics and chaos analysis of one-dimensional pulsating detonations, Combust. Theory Model. vol 9, pp. 159–170.

[6] H. D. Ng, M. I. Radulescu, A. J. Higgins, N. Nikiforakis and J. H. S. Lee (2005). Numerical investigation of the instability for one-dimensional Chapman–Jouguet detonations with chain-branching kinetics. Combust. Theory and Model. vol. 9, No. 3, pp. 385–401.

[7] A. K. Henrick, T. D. Aslam, J. M. Powers (2006). Simulations of pulsating one-dimensional detonations with true fifth order accuracy. J. Comp. Phys., vol. 213, pp. 311–329.

[8] W. Han , C. Wang and C. K Law (2019). Pulsation in one-dimensional H 2 –O 2 detonation with detailed reaction mechanism. Comb. and Flame, vol 200, pp. 242–261.

[9] M. Radulescu and J. Tang (2011) Nonlinear Dynamics of Self-Sustained Supersonic Reaction-Waves: Fickett's Detonation Analogue. Phys. Rev. Letter 107, 164503.

[10] M. Short and G. J. Sharpe (2003). Pulsating instability of detonations with a two-step chain-branching reaction model: theory and numerics. Comb. Theory and Model. vol 7 (2), pp. 401-416.

[11] J. Tang (2013). Study of the Instability and Dynamics of Detonation Waves using Fickett's Analogue to the Reactive Euler Equations. M.A.Sc. thesis, University of Ottawa (Canada).

[12] C.-W. Shu, S. Osher (1988). Efficient implementation of essentially nonoscillatory schemes for hyperbolic conservation laws, J. of Comp. Phys. vol 77 (2), 439–471.

[13] A. Sow, R. Semenko, E and A. R Kasimov (2017). On a stabilization mechanism for low-velocity detonations. J. of Fluid Mechanics. vol 816, pp. 539–553.