Detonation analogs revisited

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1 Introduction

In [14, 15], the author discussed the role played by analogs in detonation theory. The analogs were classified as "physical" and "mathematical". Physical analogs of detonations are real physical phenomena that share many similarities with detonations. For example, hydraulic jumps [13] and traffic jams [11] can be modeled as self-sustained shock waves, whose structure is very similar to that of a detonation wave in the ZND theory [10]. That is, the shock is followed by a transonic flow region, and the shock speed is determined by sonic conditions. A number of other physical analogs of detonation can be found in the literature (e.g. [1, 19]). Mathematical analogs, on the other hand, are *ad hoc* mathematical models that consist of one or more partial differential equations whose solutions behave exactly as those of the reactive Euler equations of detonation theory. The analogs are invented, not derived from first principles. The earliest and best known examples of such mathematical analogs are due to Fickett [7] and Majda [18].

Wildon Fickett introduced his analog in 1979 "for the purpose of more easily studying various topics in detonation theory" [7]. His idea was to essentially extend Burgers equation to incorporate chemical reactions so as to obtain a model that would predict chemically driven shock waves analogous to detonations. To be successful, such a model must be able to qualitatively reproduce known characteristics of detonation waves. These include: (1) traveling-wave solutions of ZND theory; (2) linear instability of these solutions when the reactions are sufficiently state sensitive; (3) existence of limit cycles beyond the stability threshold; (4) presence of period-doubling sequence of bifurcations leading to chaos; (5) ignition/failure phenomena; (6) multiplicity of steady-state solutions in non-ideal detonations; (7) existence of multi-dimensional cellular structures.

It may perhaps seem overly optimistic to hope that a simple model can capture such a rich set of phenomena. And indeed, the predictive capabilities of the original models due to Fickett and Majda were primarily limited to the steady-state one-dimensional structures. Instabilities were demonstrated for the square-wave model of detonation [9], for which the linear stability problem is ill-posed (i.e., a pathological instability is present, see also [12]). In addition, Fickett performed preliminary calculations showing that, provided the rate function is sufficiently state sensitive, the model with the rate that depends on the shock state, can result in instabilities [8]. However, he never elucidated the nature of these instabilities. In particular, no demonstration of the existence of limit cycles or period doubling bifurcations can be found in [8].

As a consequence of these findings and those based on Majda's model [18], it was generally believed that such modeling was perhaps too simplistic and therefore unable to reproduce most dynamics of detonations.

However, recent publications demonstrate that this is not so. An extension of Fickett's model that treats the chemistry as a two-stage process, wherein an induction zone is followed by a heat release zone, is capable of reproducing the dynamical richness of one-dimensional pulsating detonations [20]. Furthermore, even a scalar forced Burgers equation can be shown to capture qualitatively such diverse features of one-dimensional detonations as the ZND solutions, their linear instability, nonlinear dynamics (including chaos), ignition/failure effects, and multiplicity of solutions in non-ideal detonations [2–4, 16]. A two-dimensional extension of [16] is also possible that can be shown to reproduce the cellular dynamics of gaseous detonations [2, 6]. Thus, it seems fair to say now that the analog modeling is quite successful in representing, at a qualitative level, most essential phenomena in detonations.

Returning to Fickett's goal of "more easily studying various topics in detonation theory", a question arises as to specific benefits of such an *ad hoc* modeling for "real" problems of detonations. That is: Given that the analogs qualitatively reproduce many detonation phenomena, how does it help us understand detonations as described by the full system of reactive flow equations?

One obvious benefit of the simplified modeling is similar to that of the Burgers equation. That is, the analog can be used to simply and relatively easily illustrate the essential theoretical ideas involved in modeling detonations by physical systems of governing equations. These include the ZND theory, in which the idea of imposing sonic conditions is often non-trivial, especially in systems with multiple chemical reactions. Intricacies of linear stability analysis of detonations either by means of the Laplace transform or normal modes can also be relatively easily explained with the analog models [4]. New ideas and algorithms can be much more easily tested on the analog than on the full reactive flow system. For example, the method of transonic integration in non-ideal detonations (which can be generalized to the full Euler system) [3] is quite easy to illustrate and implement numerically with the analog model.

Development of numerical algorithms for hyperbolic systems is greatly benefitted by variety of test problems for which exact solutions are known or which are easier to implement than the full system. For example, shallow-water equations consisting of a hyperbolic system of two equations have long been used in explaining variety of algorithms in computational fluid dynamics [17]. It is well known that detonations present significant challenges for numerical algorithms in view of sensitive dependence of detonation dynamics on problem parameters and on algorithmic details. Simplified analogs that retain much of the dynamical complexity of real detonations can therefore serve as rigorous and at the same time easy to implement test problems.

Most importantly, perhaps, the ability of a simple analog to mimic much of the dynamics of real detonations is a strong motivation for the development of rational asymptotic theories of detonation that may be able to achieve the same level of predictive capabilities. Indeed, this is exactly how the recent weakly nonlinear theory [5] was developed.

2 Interplay of analogs and physical systems

To illustrate some of the details involved in analog modeling, here we summarize key mathematical ideas of detonation theory. A detonation is by definition a shock wave that is driven by chemical energy released in a combustible medium, whereby the chemical reactions are initiated as a result of the shock compression and heating. At the most basic level (i.e. when dissipative processes are neglected), detonations can be described by the reactive Euler equations which in one space dimension can be written as

$$\mathbf{u}_t + \mathbf{A}\,(\mathbf{u})\mathbf{u}_x = \mathbf{s}\,(\mathbf{u})\,, \qquad (1)$$

where $\mathbf{u} = (\rho, u, e, \lambda)^T$ is the state vector with ρ, u, e, and λ being the density, particle velocity, internal energy, and species concentration, respectively. $\mathbf{A}$ is the Jacobian of the flux vector, and $\mathbf{s}$ is the source term containing contributions from chemical reactions. As a typical example, for a one-step reaction, the species equation in this system would be $\lambda_t + u\lambda_x = \omega$, where $\omega = k\,(1-\lambda)\exp\left(-E/RT\right)$, E is the activation energy, k is the pre-exponential constant factor, and R is the universal gas constant.

If one looks for steady traveling wave solutions of equation (1) as $\mathbf{u} = \mathbf{U}\,(x - Dt)$ with the constant and unknown wave speed D, then the system becomes

$$(\mathbf{A} - D\mathbf{I})\,\mathbf{U}' = \mathbf{s}\,(\mathbf{U})\,. \tag{2}$$

The most important property of the mathematical model represented by equation (2), which is at the basis of the ZND theory of self-sustained detonations, is the possible presence of a sonic state in the flow. This occurs if the solution $\mathbf{U}$ is such that $\mathbf{A} - D\mathbf{I}$ is singular at some point in the flow (which is the sonic point by definition). Since $\mathbf{A}$ has eigenvalues u and $u \pm c$, where c is the local speed of sound, then $\mathbf{A} - D\mathbf{I}$ has eigenvalues $U = u - D$, $U \pm c$. Suppose, the wave propagates from left to right, in which case $u > 0$, $D > 0$, and $U < 0$. Then, $\mathbf{A}$ can be singular only at the point where $U + c = 0$. If such a point exists (call it x_*), the wave is called self-sustained and the point x_* is called the Chapman-Jouguet (CJ) point. A regular solution of equation (2) is obtained by demanding that $\mathbf{U}$ has no singularity at x_*. This amounts to multiplying equation (2) by the left eigenvector $\mathbf{l}_+^T$ of $\mathbf{A} - D\mathbf{I}$ corresponding to the eigenvalue $\lambda_+ = U + c$ and demanding that the left-hand side vanish at x_*, which must happen if the derivatives of the solution remain finite at x_*. Therefore, the right-hand side of that equation must vanish as well, i.e. $\mathbf{l}_+^T\mathbf{s} = 0$. These two conditions at $x = x_*$: (1) $U + c = 0$ and (2) $\mathbf{l}_+^T\mathbf{s} = 0$, serve as the regularity conditions that are needed to close the system and determine the wave speed D.

From a physical point of view, what is important in the model is that the shock evolution is governed by the dynamics of the reaction zone between the shock and the sonic point. The shock–reaction-zone coupling takes place through $C_{\pm,0}$ characteristics along which acoustic and entropy waves propagate back and forth between the shock and the sonic point, and lead to resonant amplification of the waves due to their nonlinear coupling if conditions in the reaction zone are favorable.

For the analog model to represent the same physical picture of the waves propagating from the shock into the reaction zone and back, it is in general necessary to have at least two equations representing two characteristic speeds. For example, the Fickett's model,

$$u_t + uu_x = -q\lambda_x, \tag{3}$$
$$\lambda_t = \omega(u,\lambda), \tag{4}$$

in characteristic form is given by

$$u\frac{du}{dt} + q\frac{d\lambda}{dt} = q\omega, \quad \text{on} \quad \frac{dx}{dt} = u, \tag{5}$$
$$\frac{d\lambda}{dt} = \omega, \quad \text{on} \quad \frac{dx}{dt} = 0, \tag{6}$$

and shows that, for the wave that propagates from left to right with $u > 0$, C_+ characteristic, given by $dx/dt = u$, propagates toward the shock, while the other characteristic, C_0 say, does not propagate in the given laboratory frame of reference, $dx/dt = 0$, but it does propagate away from the shock. The communication among these waves and the shock is the main physical process that is responsible for the self-sustained propagation of the shock in (3-4).

It is well known that (3-4) does faithfully represent the steady-state ZND structure of detonations and a number of other steady-state phenomena in detonations [8]. However, whether the system admits the same instabilities as those present in the reactive Euler equations, remained unclear until recently.

The first resolution of this questions was proposed in [20], where the following extension of Fickett's model was analyzed,

$$\begin{aligned} u_t + uu_x &= -q\lambda_{r,x}, & (7)\\ \lambda_{i,t} &= -K_i H(\lambda_i) \exp\left[\alpha \frac{\rho}{2D} - 1\right], & (8)\\ \lambda_{r,t} &= K_r \left[1 - H(\lambda_i)\right] (1-\lambda_r)^{\nu}. & (9) \end{aligned}$$

Here H is the Heaviside function, K_i, K_r are rate constants, ν is the reaction order, and α is the sensitivity parameter analogous to the activation energy. The induction period is described by function λ_i which varies from 1 at the shock to 0 at the end of the induction period. When $\lambda_i = 0$ is reached, the heat release process begins following (9), such that λ_r increases from 0 at the tail of the induction zone to 1 at the end of the heat-release region. This model is shown in [20] to predict a sequence of period-doubling bifurcations as the parameter α is increased. The larger α implies increased sensitivity of the induction period to variations of the shock state.

In [5], the authors proposed that a simple choice of the rate function in the original model of Fickett can also reproduce the unstable dynamics of detonations. The choice of the new function is motivated by asymptotic developments in [5], which suggest that, in order to represent the physics of instability, the rate function should likely have its dependence on λ such that the rate achieves a maximum inside the reaction zone. In particular, if ω is taken in the form, $\omega = k(1-\lambda)\exp(au + b\lambda)$, with positive parameters a and b, then the Fickett's model

$$\begin{aligned} u_t + uu_x &= -\lambda_x, & (10)\\ \lambda_t &= -k(1-\lambda)\exp\left(au + b\lambda\right), & (11) \end{aligned}$$

can be shown to contain instabilities provided that, e.g. a is large enough at a fixed $b > 0$.

Perhaps, the ultimate simplification is provided by the model given in [16], which consists of a single scalar equation given by

$$u_t + uu_x = f\left(x - x_s(t), \dot{x}_s(t)\right), \quad (12)$$

where f is a forcing term that depends on the shock position, x_s, its speed, $\dot{x}_s$, and the distance to the shock, $x - x_s$. It is assumed that $f = 0$ at $x > x_s$, that f achieves its maximum value some distance from the shock, and that it decays to zero sufficiently fast far from the shock. These properties of f are motivated by the desire to make f behave like the rate of reaction in real detonations.

In [4], equation (12) is shown to precisely mimic essentially all characteristics of one-dimensional planar detonations. It not only contains the ZND-like theory of steadily propagating detonations, but also all elements of detonation linear stability theory, including various issues with radiation conditions, and nonlinear dynamics involving the period-doubling transition to chaos. It can also be easily extended to capture many other detonation phenomena, including cell formation in multiple spatial dimensions [3,6].

The model in [4, 16] points out that instabilities can arise as a result of wave amplification in a resonant-cavity-like reaction zone, such that slow waves propagating along the forward characteristics of the reactive Burgers equation interact with the shock and the fast waves propagating away from the shock into the reaction zone. The more sensitive the size of the cavity is to the state at the shock and the faster the energy is released compared to the induction time, the more unstable the system is.

3 Conclusions

Recent developments of the analog modeling of detonations originally introduced by Fickett have succeeded in reproducing many dynamical features of detonations [3, 4, 6, 16, 20, 21]. It is shown, for example, that a simple hyperbolic system of two partial differential equations is capable of predicting steady-state traveling wave solutions, their linear instability, and nonlinear dynamics that are in close qualitative agreement with corresponding properties of detonations in the reactive Euler equations.

These results have a number of important implications for understanding detonations. The analog models help elucidate the ideas and tools involved in describing various features of detonations, such as sonic points, radiation conditions, multiplicity of solutions, instabilities, bifurcations, and others. They highlight important effects responsible for particular trait in detonation structure and dynamics, which can guide in theoretical developments in detonations within the framework of reactive Euler or Navier-Stokes equations. Mathematical analog modeling is also helpful in getting insights into mechanisms of physical analogs of detonations, whose theoretical description can be guided by the understanding achieved with detonations. The analog models of detonations can be helpful in understanding the variety of mathematical questions about hyperbolic systems sharing the same properties, namely the existence and nature of instabilities, bifurcations, and complex attractors. Finally, these simple models can be helpful as test systems for the development of numerical algorithms for hyperbolic systems.

References

[1] A. V. Emelianov, A. V. Eremin, A. A. Makeich, and V. E. Fortov. Formation of a detonation-like condensation wave. *JETP Letters*, 87(9):470–473, 2008.

[2] L. M. Faria. *Qualitative and Asymptotic Theory of Detonations*. PhD thesis, King Abdullah University of Science and Technology, 2014.

[3] L. M. Faria and A. R. Kasimov. Qualitative modeling of the dynamics of detonations with losses. *Proceedings of the Combustion Institute*, 35:2015–2023, 2015.

[4] L. M. Faria, A. R. Kasimov, and R. R. Rosales. Study of a model equation in detonation theory. *SIAM Journal on Applied Mathematics*, 74(2):547–570, 2014.

[5] L. M. Faria, A. R. Kasimov, and R. R. Rosales. Theory of weakly nonlinear self-sustained detonations. *arXiv preprint arXiv:1407.8466*, 2014.

[6] L. M. Faria, A. R. Kasimov, and R. R. Rosales. A toy model for multi-dimensional cellular detonations. In *25th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS)*, Leeds, UK, 2015.

[7] W. Fickett. Detonation in miniature. *American Journal of Physics*, 47(12):1050–1059, 1979.

[8] W. Fickett. *Introduction to Detonation Theory*. University of California Press, Berkeley, CA, 1985.

[9] W. Fickett. Stability of the square-wave detonation in a model system. *Physica D: Nonlinear Phenomena*, 16(3):358–370, 1985.

[10] W. Fickett and W. C. Davis. *Detonation: theory and experiment*. Dover Publications, 2011.

[11] M. Flynn, A. R. Kasimov, J.-C. Nave, R. Rosales, and B. Seibold. Self-sustained nonlinear waves in traffic flow. *Phys. Rev. E*, 79(056113), 2009.

[12] F. S. Hall and G. S. S. Ludford. Stability of a detonation wave. *Physica D: Nonlinear Phenomena*, 28(1-2):1–17, 1987.

[13] A. R. Kasimov. A stationary circular hydraulic jump, the limits of its existence and its gasdynamic analogue. *J. Fluid Mech.*, 601:189–198, 2008.

[14] A. R. Kasimov. Detonation analogs. In *22nd International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS)*, Minsk, Belarus, 2009.

[15] A. R. Kasimov. On detonation analogs. In *23nd International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS)*, Irvine, CA USA, 2011.

[16] A. R. Kasimov, L. M. Faria, and R. R. Rosales. Model for shock wave chaos. *Physical Review Letters*, 110(10):104104, 2013.

[17] R. J. LeVeque. *Finite volume methods for hyperbolic problems*. Cambridge University Press, 2002.

[18] A. Majda. A qualitative model for dynamic combustion. *SIAM Journal on Applied Mathematics*, 41(1):70–93, 1980.

[19] M. Modestov, V. Bychkov, and M. Marklund. Ultrafast spin avalanches in crystals of nanomagnets in terms of magnetic detonation. *Physical Review Letters*, 107(20):207208, 2011.

[20] M. I. Radulescu and J. Tang. Nonlinear dynamics of self-sustained supersonic reaction waves: Fickett's detonation analogue. *Phys. Rev. Lett.*, 107(16), 2011.

[21] J. Tang and M. Radulescu. Dynamics of shock induced ignition in Ficketts model: Influence of χ. *Proceedings of the Combustion Institute*, 2012.