On detonation analogs

Aslan Kasimov
King Abdullah University of Science and Technology
Thuwal, Saudi Arabia

2 Introduction

An analog is important as a simplified tool that can shed light on certain qualitative features of a complex phenomenon which are otherwise hard to understand. Detonation is certainly a very complex phenomenon: (i) it is difficult to study experimentally due to extreme conditions that exist in it, such as very high flow speeds, pressures, and temperatures; (ii) it is difficult to calculate numerically due to extremely fine resolutions it requires, sophisticated algorithms it demands, and large disparity of time and length scales it involves; (iii) it is difficult to analyze theoretically due to the nature of the underlying set of hyperbolic balance laws with strongly nonlinear and stiff source terms. A good analog model would be helpful in understanding various problems in detonation, in particular, pulsations of one-dimensional detonations, formation and propagation of cellular detonations, initiation of detonation either by a strong source or through a transition from deflagration.

Fickett [4] and Majda [13] independently and at about the same time around 1980 introduced the first detonation analogs. The principal idea behind them is the desire to construct a mathematical model that would be as beneficial to detonation (and combustion) theory as the Burgers' equation is to fluid dynamics. Just like the Burgers' equation became a prototype for introducing the concepts of characteristics, shocks, rarefactions, and entropy conditions that are so important in gasdynamics and in the theory of hyperbolic partial differential equations, the hope was that detonation analog would be able to reproduce, at least on a qualitative level, the basic features of classical CJ and ZND theories [8]. Indeed, the models of Fickett and Majda have been shown to reproduce many aspects of the classical theories. Yet such important phenomena as the pulsating instability, cell formation, ignition and failure, and deflagration-to-detonation transition remain outside the capabilities of these analogs.

It must be emphasized that the analogs by Fickett and Majda have been *designed* in an *ad hoc* way, not derived rationally from reactive flow equations (although, in a later paper by Rosales and Majda [14] these models were shown to arise in a certain asymptotic limit from the full combustion system). The main idea was to construct a mathematical analog which may not necessarily describe a real physical system, but nevertheless posesses necessary complexity to be able to reproduce some reality of detonations. The *ad hoc* nature of the analogs does certainly limit their value in comparison to, for example, asymptotic theories which originate from the underlying system of governing equations. Nevertheless, as studies of Fickett's (and Majda's) analog have shown, there is much insight that one can gain from their analysis (see, e.g. [2, 5, 6]).

Correspondence to: aslan.kasimov@kaust.edu.sa

In contrast to this *ad hoc* approach, there exists another one where one looks for real physical phenomena that are similar in some respects to, but are simpler than detonation. In this approach, the mathematical analog is not designed or invented, but is taken from a rational description of the analog physical system. The analysis of the simpler physical problem is then carried out with a specific aim at elucidating the more complicated problem. We mention two well-known phenomena that can be considered as detonation analogs [11]: the hydraulic jump in shallow-water theory [10] and the traffic jam in second order continuum theories of traffic [9].

In the following sections we discuss in some detail how the analogs are similar to detonations and what their strengths and limitations are.

3 Essential features of detonation

A detonation is a shock wave that is sustained by the chemical energy released in the post-shock reaction zone. The reactions are themselves sustained by high temperatures caused by the shock compression. The presence of a shock wave means that the phenomenon is described by a nonlinear hyperbolic system (Euler equations) and the presence of chemical reactions implies strongly nonlinear (exponential) sensitivity of the energy release to local thermodynamic state. Thus a detonation is characterised by a strong coupling of these two highly nonlinear phenomena. An analog must account for this coupling in order to be faithful to the essential nature of detonation.

A special class of self-sustained detonation waves is of most practical and theoretical relevance and is hardest to analyze mathematically and calculate numerically. Such detonations are described by a singular set of reactive Euler equations, where the singularity occurs due to the transonic nature of the post-shock flow.

In order to illustrate this idea better, consider the reactive Euler equations in one dimension,

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

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 the chemical reaction rates. 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, k pre-exponential constant factor and R the universal gas constant.

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

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

As long as $\mathbf{A} - D\mathbf{I}$ is nowhere singular, this system can be solved relatively easily between the shock, where the Rankine-Hugoniot conditions must be imposed, and the far field with whatever conditions are demanded there. Clearly, the latter conditions are not immediately obvious, but they are necessary in order to determine the wave speed D, since the number of jump conditions is the same as the number of components of $\mathbf{U}$ while D is an extra unknown.

An important special case occurs if the solution is such that $\mathbf{A} - D\mathbf{I}$ can become singular at some point in the flow. Since $\mathbf{A}$ has eigenvalues u, and $u \pm c$, where c is the local sound speed, then $\mathbf{A} - D\mathbf{I}$ has eigenvalues $U = u - D$, $U \pm c$**.** Suppose the wave propagates from right to left, 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_c), the wave is called self-sustained and the point x_c the Chapman-Jouguet point. A regular solution of (2) is obtained by demainding that $\mathbf{U}$ has no singularity at x_c[1]. This amounts to multiplying (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_c. Therefore, the right-hand side of that equation must vanish as well, i.e. $\mathbf{l}_-^T\mathbf{s} = 0$. These two conditions at $x = x_c$: 1) $U - c = 0$ and 2) $\mathbf{l}_-^T\mathbf{s} = 0$, serve as the far-field boundary conditions that are needed to close the system and determine the wave speed D. Note that these are intrinsic boundary conditions coming from a regularity requirement. They are not imposed externally as would be the case, for example, in a piston-supported detonation.

An analog that is true to the nature of a self-sustained detonation has necessarily to be represented by a hyperbolic system having the properties discussed in the previous paragraph. The simplest such system would consist of two equations with two characteristic speeds, one of which can vanish at a sonic point. Indeed, the two examples that we discuss below (hydraulic jump and traffic jam) do posess this property and are good candidates as detonation analogs. Since the original Euler system consists of at least four equations with two acoustic and two entropy characteristics, there is an opportunity to build a more complex analog that can represent two acoustic and one entropy fields and be able to predicts richer set of phenomena than a two-equation analog can.

4 Mathematical analogs of detonation

Mathematical analogs are best described by the quote from Fickett [4]: “An analog is a *qualitative* representation of the original... The analog is constructed or designed, not derived. The design involves a trade off: one tries to maximize the simplicity while minimizing the loss of important properties of the original. Simplicity is the analog’s strong point. Specifically: (i) exact solutions are easier to find and more likely to exist, (ii) the tedium of routine mathematical manipulations is greatly reduced, and (iii) the essential ideas are less likely to be obscured by extraneous detail−in the full system one may fail to the see the forest for the trees.”

The analog of Fickett [4] is designed with ideas that parallel the development of the traffic flow theory by Lighthill and Whitham [12, 15]. Similar to the assumption of their kinematic traffic theory, that the flux ρu in the equation for the conservation of the number of cars, $\rho + (\rho u)_x = 0$, depends on density ρ only, Fickett’s theory assumes that the flux $p = \rho u$ in his detonation analog, $\rho_t + p_x = 0$, depends on density. In order to account for the role of chemistry, he assumes additionally that p also depends on the reaction variable λ. Consequently, a second equation is necessary to determine λ. This equation is taken as $\lambda_t = \omega$ that comes from the true rate equation by throwing out the convective term. The final step is then to close the system by adding constitutive relations, which are taken, for example, as $p = \frac{1}{2}(\rho + q\lambda)^2$ and $\omega = k\sqrt{1-\lambda}$, where q is the “heat of reaction” and k is rate constant. As shown by Fickett in his subsequent work [2, 3, 5–7], the model does predict many qualitative features of real detonation waves. It seems fair to say that Fickett’s analog has played its role in detonation similar to that of Burgers’ equation in fluid dynamics or the kinematic wave equation, $\rho + (Q(\rho))_x = 0$, in traffic flow theory.

Majda’s analog system [13] consists of the following two equations: $\rho_t + f_x = \beta\rho_{xx} - q_0\omega$ and $\lambda_t = \omega$, where $f = f(\rho)$ is a convex flux, $\omega = K\phi(\rho)\lambda$, q_0, K are constants, and ϕ is the rate function. The system resembles Fickett’s analog very closely with the difference due to the diffusion (unimportant in detonation) and reaction terms in the advection equation.

[1] Strictly speaking, this is not necessary. We only require that $\lim_{x\to x_c}\left(\lambda_- \mathbf{l}_-^T\mathbf{U}'\right) = 0$.

5 Physical analogs of detonation

While the mathematical analogs have their merit as argued above, there is another class of analogs that do not fit into Fickett's definition. These are analogs that are derived, not designed, but they are derived for a completely different physical system that may have nothing to do with the original. The roots of the analogy then stem from the similarity of the underlying governing equations between the original and the analog.

Two examples we mention here (there are others) are a circular hydraulic jump and traffic flow. The hydraulic jump can be described to a good approximation by the shallow-water equations consisting of the depth-averaged continuity and radial momentum equations:

$$h_t + (hu)_r = -\frac{hu}{r}, \tag{3}$$

$$u_t + uu_r = -gh_r + gs_b(r) - gs_f(h,u), \tag{4}$$

where r is the radial distance, h is the fluid depth, g is the constant of gravity, and u is the radial velocity. The source terms in the momentum equation come from the slope of the bottom topography $s_b(r)$ and the friction slope s_f. The system is hyperbolic and has the same structure as (1). Importantly, there exists a steady-state radially symmetric solution with a shock for a problem with a radial flow source at $r = 0$. The structure of this solution can be found following exactly the same ideas as in the discussion above for the self-sustained detonation. That is, the hyperbolic system is solved subject to jump conditions at the shock and CJ conditions at the sonic point, which must exist in order for the problem to be well-posed [10]. The difference here is that the hyperbolic system only posesses two acoustic families of characteristics.

A similar analog exists in an extension of the continuum theory of traffic flow of Lighhill and Whitham [12, 15]. Again, the governing equations are hyperbolic balance laws:

$$\rho_t + (\rho u)_x = 0, \tag{5}$$

$$u_t + uu_x = -\frac{1}{\rho}p_x + \frac{1}{\tau}(\tilde{u}(\rho) - u), \tag{6}$$

where $\tilde{u}(\rho)$ is the so-called "desired velocity", which is a given function of density, and $p(\rho)$ is the traffic "pressure", typically taken as $p = \beta\rho^n$ as in a polytropic fluid. The system is again of the form (1) and again admits traveling wave solutions $\mathbf{u} = \mathbf{U}(x - Dt)$. When the solution is a shock wave, it is analogous to the CJ solution of detonation theory due to the fact that a sonic point can exist in the flow. A regularity requirement at the sonic point leads to a unique solution of the problem. A typical profile of the vehicle number density in a traffic jam is shown in Fig. 1 with its striking resemblance of a detonation structure.

The most interesting and difficult problems in detonation theory are associated with instabilities, other transients, and multi-dimensionality. None of the above analogs can at present adequately represent these features. However, based on observations, the hydraulic jump instabilities may be close to those of detonations. Experimentally, hydraulic jumps can be seen to undergo not only longitudinal (pulsating) instabilities as in undular jumps, but also transverse instabilities leading to triple points as in cellular detonations, see Fig. 1. The problem with this analog is that no simple analysis currently exists that explains the formation of the polygonal structures. Nevertheless, we believe it is worthwhile to study these problems as they are still simpler than detonations and the tools developed in their studies may find their use in detonation analysis.

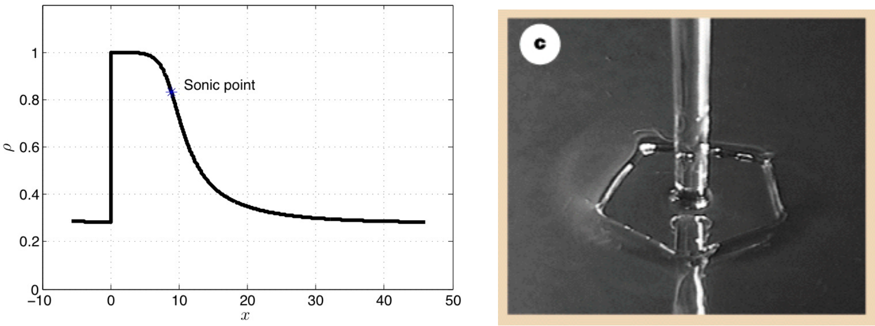

Figure 1: ZND-like structure of a traffic jam (left, [9]). A polygonal hydraulic jump (right, [1]).

6 Conclusions

We discussed two classes of detonation analogs distinguished by their origin. One class, that was originally introduced by Fickett, is an *ad hoc* mathematical construct akin to Burgers' equation that captures certain features of detonations. Analogs in this class are purely mathematical inventions and may have no physically realistic phenomenon behind them. Nevertheless, cleverly constructed (as the Fickett's analog is), these analogs may be able to capture many realistic features of detonations qualitatively well.

The second class of analogs has a very different origin. They come from a real physical phenomenon, but one which at first sight appears to have nothing in common with detonation. We discussed two such analogs: traffic jam and hydraulic jump. The analogy of these phenomena with detonation stems from the comparison of the underlying hyperbolic systems. In all cases, the systems are balance laws that admit traveling shock-wave solutions of self-sustained nature so that the wave consists of a shock followed by a transonic flow. The existence of a sonic point is the key factor in the analogy between these simpler phenomena and the self-sustained detonation.

Ultimately, the goal of this effort is to understand the nature of detonation. While theoretical (e.g. asymptotic) and numerical tools are also available in pursuing this goal and will generally be preferable since they deal directly with the underlying reactive Euler equations, we believe there is still much value in studying simpler analogs which may help to "see the forest for the trees."

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