Dynamic Behaviour of Analog Detonation Systems

Kiyanda, C.B.¹ and Ng, H.D.² ¹Los Alamos National Laboratory Los Alamos, U.S.A. ²Concordia University Montreal, Canada

1 Introduction

Systems analogous to compressible flow have long been studied. The Burgers' equation is often used as a prototype, non-linear, hyperbolic system which has a single characteristic and accepts rarefaction and shock solutions [12]. The shallow-water wave equations, i.e. the long-wave approximation of freesurface, gravity flows, is also a hyperbolic system with shock and rarefaction solutions analogous to those of compressible fluid flows. Since shallow-water flow describes a physical system, visualization of experiments is possible and water tables have been used in the past to study the behaviour of supersonic flow around two-dimensional objects such as diamond airfoils and also to demonstrate the irregular or Mach reflection [6]. The hydraulic analogue to detonation waves has also been used early on by Oppenheim to investigate the structure of detonation waves [8,9].

Analogs to the basic components of supersonic fluid flows (i.e. shock waves and rarefactions) have counterparts in the analog systems as well and these analog models can be extended to mimic the behaviour of reactive systems as well, including detonation waves. A detonation analog model derived by Fickett [4] was used in the now known *Introduction to Detonation Theory* [5] to carefully outline the basics of detonation theory. Fickett thereby established that the steady detonation structure in his model is analogous to that of detonations in an Euler world. Clarke et al. carried numerical simulations of the Fickett model, looking at the initiation dynamics [3] and found no oscillatory solutions. Recently however, Radulescu and Tang observed a pulsating instability of Fickett's model with a period-doubling bifurcation [10]. A similar model was formulated as an asymptotic model for the Euler equations by Majda [7, 11] and used as a numerical test problem by Bourlioux [2]. For the Majda model, no unstable solutions were observed. Recently, Barker and Zumbrun concluded from stability analysis that Majda's model does not support instabilities for Arrhenius kinetics [1].

In the present work, we seek to construct a hierarchy of detonation analogs using the Burgers' and shallow-water wave equations as basic building blocks. The formulated models should exhibit different combustion regimes analogous to those of an Euler gas, i.e. "detonation"-like and "constant volume combustion"-like solutions. The questions we ask pertain to the dynamic behaviour of detonation waves in those analog models. While we know these models admit a detonation solution, under what conditions can this detonation solution be unstable and oscillate? What is then the basic mechanism for instability? We will construct two different analog models which we investigate both using numerical simulations

and theoretically by looking at the linear stability analysis. The influence of the choice of reaction kinetics will be investigated.

2 Description of the Analog Systems

When constructing the analog systems, we insist on some basic properties:

- 1. the system must have features analogous to shock waves and rarefaction waves,
- 2. the system must admit a detonation solution,
- for spatially uniform initial conditions, the system must admit a solution analogous to a "constant volume" reaction process.

Condition 1 is automatically satisfied by our use of the Burgers' and shallow-water wave models as basic building blocks. Both models admit shock-like and rarefaction-like solutions. Condition 2 will be easily shown to be satisfied and the steady 1D detonation solution will be derived. The necessity for those first 2 conditions is self-evident. Finally, while condition 3 is easily shown to be true for a given model, the reason for imposing such a condition will only be apparent later.

The first model we construct consists of a Burgers' model with an added reactive term

$$\frac{\partial h}{\partial t^{\rm l}} + h \frac{\partial h}{\partial x^{\rm l}} = Q \Sigma r_i q_i, \tag{1}$$

$$\frac{\partial \lambda_i}{\partial t^1} = r_i; \tag{2}$$

In conservative form, 1 becomes $[h - Q \sum q_i \lambda_i]_{t^l} + [h^2/2]_{x^l} = 0$ and the model is close to Majda's model [7]. Our reactive Burgers' model differs slightly from the Fickett model

$$\frac{\partial h}{\partial t^{\rm l}} + \frac{1}{2} \frac{\partial}{\partial x^{\rm l}} \left(h^2 + \lambda q \right) = 0, \tag{3}$$

$$\frac{\partial \lambda}{\partial t^{\rm l}} = r. \tag{4}$$

While both models sustain detonation solutions, our model results in a reactive model for spatially uniform flows, mimicking a constant volume explosion with a finite generation of the scalar quantity h. This satisfies condition 3. Fickett's model, for a spatially uniform initial condition, will allow the reaction to progress, but *no amount of* h will be produced. Furthermore, the reactive term in Fickett's model is of the form $qd\lambda/dx$, which means that the scalar quantity h can be either generated or consumed depending on the local distribution of λ . Hence, a rarefaction wave propagating into a uniform flow will result in a locally endothermic process within the region affected by the rarefaction, while the region yet unaffected by the rarefaction will be thermally neutral.

The second model we construct is based on the shallow-water wave approximation augmented by a volumetric "height addition" term.

$$\frac{\partial h}{\partial t^{\rm l}} + \nabla^{\rm l} \cdot (h\underline{u}) = Q\Sigma r_i q_i, \tag{5}$$

$$\frac{\partial (h\underline{u})}{\partial t^{l}} + \nabla^{l} \left(h\underline{u} \cdot \underline{u} + \frac{1}{2}gh^{2} \right) = 0, \tag{6}$$

$$\frac{\partial \lambda_i}{\partial t^1} + \underline{u} \cdot \nabla^1 \lambda_i = r_i. \tag{7}$$

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The detonation solution will be shown to exist in the next section and, again, it is easily shown that a spatially uniform initial condition results in a constant-volume like combustion.

The formulation of two different models allows the construction of an analog system hierarchy based on the number of characteristic waves present. The unreactive Burgers' system exhibits only 1 characteristic direction, i.e. only a forward-facing characteristic is present. In the Burgers' system, one can think of the lines of constant x as particle paths which are always stationary. The reactive shallow-water wave analog has both backward facing and forward facing characteristics, making this model much closer to the Euler system. The Euler system has yet an additional characteristic wave, i.e. the entropy characteristic. We can therefore observe detonation waves in systems with increasing complexity.

3 ZND Detonation Structure

3.1 Reactive Burgers'

For the reactive Burgers' system, the steady detonation velocity is given by $D = Q + h_0 + \sqrt{Q(Q + h_0)}$, where h_0 is the initial, "quiescent" value of h. The von Neumann and CJ states are $h_{vn} = 2D - h_0$ and $h_{cj} = D$ with $\lambda = 0$ for the unreacted state and 1 for the reacted state. The states through the reaction zone are given by $h(\lambda) = D + \sqrt{D^2 - \beta^2}$, where $\beta^2 = D^2 - (D - h_0)^2 + 2DQ\lambda$.

In the case of a single-step model, the location of the maximum of h can be shown to always be at the shock. The derivative of h with x (in the reference frame of the shock where $x \le 0$) is

$$\frac{dh}{dx}|_{x=0} = \frac{rQ}{D-h_0} \tag{8}$$

and h can only increase near the shock for $r(\lambda = 0) < 0$. For a reaction rate of the form $r = (1-\lambda)f(h)$ the detonation profile can only have a maximum of h away from the shock if $f = f(h, \lambda)$ and is non-monotonic or if the mass fraction λ is allowed to be negative.

A 2 sequential step model, $A \to B \to C$, allows the wave to exhibit an initial endothermic step and hence a maximum of h away from the front while imposing that $\lambda_1, \lambda_2 \in [0, 1]$, as in the 2-step Arrhenius models

$$\frac{\partial \lambda_1}{\partial t^l} = r_1 = k_1 (1 - \lambda_1) e^{-h_1/h} - k_2 \lambda_1 e^{-h_2/h}, \tag{9}$$

$$\frac{\partial \lambda_2}{\partial t^1} = r_2 = k_2 \lambda_1 e^{-h_2/h},\tag{10}$$

with $q_1 < 0$ and $q_2 > 0$.

3.2 Reactive Shallow-Water Wave

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Hydraulic jumps in the shallow-water wave model are equivalent to shock waves in a compressible gas and "shock relations" are easily derived between an initial state($_1$) and a shocked state ($_2$), s.t.

$$u_1^2 = \frac{1}{2}g\frac{h_2}{h_1}\left(h_2 - h_1\right) \tag{11}$$

Dynamic Behaviour of Analog Detonation Systems

or

$$h_2 = \frac{h_1}{2} + \sqrt{\frac{h_1^2}{4} + \frac{2u_1^2 h_1}{g}}.$$
(12)

The differential equations controlling the znd structure are

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$$\iota_x = \frac{\left(u^2 + gh\right) Q\Sigma r_i q_i}{h \left[ah - u^2\right]},\tag{13}$$

$$h_x = -2\frac{uQ\Sigma r_i q_i}{gh - u^2},\tag{14}$$

$$(\lambda_i)_x = \frac{r_i}{u}.$$
(15)

For a single-step reaction rate, it can be shown the reactive shallow-water wave model must also only accept solutions for which h is an extremum at the front. A 2-step reaction rate with a endothermic first step allows the variation of h through the reaction zone structure to be non-monotonic and hence maximum some distance away from the lead shock.

4 Numerical Simulations of Reactive Burgers' Model

Preliminary simulations were performed on the reactive Burgers' model. A basic numerical scheme was used consisting of an explicit 1st order in time and 1st order source term splitting integration with an exact Riemann solver. For the Burgers' model with $h(x) \ge 0$ everywhere, the exact solution to the Riemann problem is always $h = h_L$ and is computationally trivial. The initial conditions used were analogous to a local high pressure region. The initial value of the scalar h was set to a high value $h = h_0$ for $x < x_0$ and h = 0 otherwise. The left boundary condition was a piston at h = 2 and $\lambda = 0$, corresponding to the CJ sonic conditions. We first computed the solution by assuming a single step Arrhenius reaction with $r = k\lambda e^{-h_a/h}$. The activation scalar, h_a was varied over 3 orders of magnitude, $0.1 \le h_a \le 10$, while the pre-exponential constant was fixed at k = 10 unless stated otherwise. The domain, of a length of 50 units, contained 3000-5000 computational cells, which always resulted in a minimum of 60 cells through the half-reaction zone length. Hereafter, we report the history of the shock front amplitude as a function of the location of the shock as our main diagnostic of the wave behaviour.

Over the range $0.1 \le h_a \le 2.0$, a detonation was initiated and the resulting wave appears to be stable, as shown in fig 1. The dynamic behaviour consists of an initial shock acceleration caused by the burning of the "high-pressure" region, followed by a monotonic decay to the detonation solution.

For a higher value of the activation energy, $h_a = 10$, variations in the extent of the initial "high-pressure" region reveals different initiation dynamics of the wave, as shown in fig 2. For larger initiation regions, the initial wave acceleration is followed by a steady decay. The two smaller initiation region tested, $x_0 = 1,5$ yield 3 distinct phases in the initiation region. First, a wave acceleration, followed by a decay from the left expansion wave finally followed by a monotonic re-acceleration (shown for $x_0 = 1$). Simulations of the equivalent conditions with k = 100 (equivalent to simulating a longer domain) show that all three cases asymptote to the steady detonation solution.

Given these very preliminary results, it appears as though, over a range of 2 orders of magnitude, the reactive Burgers' model with a single-step Arrhenius reaction rate is stable. The fact the equivalent Euler system can in fact exhibit unsteady solutions would suggest the existence of a rear-facing characteristic is necessary for the detonation to be unstable. This exact question will be answered by further,



Figure 1: Stable solutions with a single step, Arrhenius kinetic and $0.1 \le h_a \le 2.0$.



Figure 2: Two different initiation behaviours with $h_0 = 6$ over different region sizes $1 \le x_0 \le 10$.

more in-depth, numerical examination of the reactive Burgers' and reactive shallow-water wave models. The linear stability analysis of these models will also give a definite answer in the event that unstable solutions, in fact, do exist for this class of models.

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