Detonation in Miniature

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ABSTRACT

A simple mathematical analog for reactive flow is proposed: a kinematic wave equation like the Burgers or Korteweg-deVries equation, which has the necessary properties for application to detonation. Also given is a tentative table of contents of a proposed short book covering much of reactive flow and detonation theory "in miniature," that is, with discussion of properties and solutions of this analog and its variants.

The prototype is inviscid reactive flow with particular application to detonation. The simplest form of the proposed analog is

\[ \rho_t + p_x = 0 \]  
\[ \lambda_t = r \]  
\[ p = p(\rho, \lambda) = (\rho + q\lambda)^{1/2} \]  
\[ r = r(\rho, \lambda) \]

Although this is not a physical model, for convenience of discussion we use the standard terms of reactive flow and detonation theory, with symbols as follows:

- \( x \) = position
- \( t \) = time
- \( p \) = pressure
- \( \rho \) = density
- \( \lambda \) = degree of reaction
- \( r \) = reaction rate
- \( q \) = heat of reaction
- \( c \) = frozen sound speed.

We have the equation of motion or conservation law [Eq. (1)], the rate equation [Eq. (2)], the equation of state [Eq. (3)], and the rate function [Eq. (4)]. The shock jump relations are

\[ [p]/[\rho] = U \]  
[\[ \lambda \] = 0 , \]

where \( U \) is the shock velocity and the brackets denote a jump.

Compared to the prototype, the analog's most serious lack is the absence of left-facing waves. However, it has the other important properties and is a much simpler system to analyze. It has the usual partial-reaction Hugoniot system with the standard sonic properties and topology, so that there are weak and strong branches and a Chapman-Jouguet condition for the unsupported detonation.

For the particular equation of state of Eq. (3), Eqs. (1)-(4) can be written

\[ c_t + cc_x = qr \]  

\[ \lambda_t = r \]
\[ r = r(c - q\lambda, \lambda) \]
\[ c = \rho + q\lambda = (\partial p/\partial \rho)_\lambda . \]

In characteristic form these are
\[ \frac{dc}{dt} = qr \quad \frac{d\lambda}{dt} = c \]
\[ \frac{d\lambda}{dt} = r \quad \frac{dx}{dt} = 0 . \]

Note that the forward characteristics move at frozen sound speed. A solution steady in a frame moving with constant velocity \( U \) satisfies
\[ \frac{d(p + \rho U)}{dy} = 0 \]
\[ \frac{d\lambda}{dy} = r/U \]
\[ y = x - Ut . \]

The ZND model of a detonation consists of a shock followed by a steady reaction zone. Let the initial state be \( p = p_0, \rho = \rho_0, \lambda = 0 \). Integrating the steady-solution equation [Eq. (13)] and combining with the jump relation [Eq. (5)] gives the Rayleigh line along which the steady solution must lie,
\[ p - p_0 = U(p - p_0) . \]

Using the equation of state [Eq. (3)] for \( p \) in this equation gives \( \rho \) as a function of \( \lambda \) through the steady solution
\[ \rho = U - q\lambda + \left[ U^2 - 2(q\lambda + 1)U + 1 \right]^{1/2} , \]
where we have taken \( \rho_0 = 1 \). The spatial profile \( \rho(y) = \rho(\lambda(y)) \) is obtained by integrating the rate equation [Eq. (14)].

Two Rayleigh lines and the partial-reaction Hugoniots for \( \lambda = 0 \) and \( \lambda = 1 \) are shown in Fig. 1. Because the characteristic speed is the slope of the partial-reaction Hugoniot and the shock speed is the slope of the Rayleigh line, we see that an upper intersection like point \( S \) is subsonic (characteristic speed greater than shock speed), a lower intersection like point \( W \) is supersonic (characteristic speed less than shock speed), and the tangent or Chapman-Jouguet point \( J \) is sonic. The Chapman-Jouguet velocity is obtained by setting the radical in Eq. (17) to zero (with \( \lambda = 1 \),
\[ U_j = (q + 1) + [(q + 1)^2 - 1]^{1/2} \]
\[ \rho_j = U_j - q . \]

Variations on Eqs. (1)-(4) will allow us to cover most of detonation theory. We can use different forms of the reaction rate and the equation of state, add more reactions, and modify the equation of motion by adding a viscous term. To show the range of applications, we give a table of contents for a proposed short book in Table I.
TABLE I
PROPOSED TABLE OF CONTENTS

1. The Model

2. Properties of the Equations
   Characteristics/ jump relations/ steady solutions/
   dispersion relations/ variable transformations

PART I. STEADY AND APPROXIMATELY
SELF-SIMILAR SOLUTIONS

3. Equilibrium Initial State
   Shocks/ acceleration waves

4. Metastable Initial State (Detonations)
   One-reaction irreversible*/ one-reaction
   reversible*/ two-reaction irreversible/ two-
   reaction reversible/ viscous/ phase
   transformation

5. Hydrodynamic Stability of the Steady
   Solution
   Shock (non-reactive)/ square wave/ one-reaction
   irreversible/ viscous

PART II. NONSTEADY SOLUTIONS

6. Exact Solutions

7. Finite-Difference Calculations

*"Irreversible" here means forward reaction only; "reversible"
means forward and back reaction with an equilibrium \( \lambda \) which is
in general a function of \( \rho \).