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Properties of Detonation Waves

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1 Summary

The phenomenon of unphysical wave propagation speeds sometimes occurs in numerical computations of detonation waves on coarse grids. The strong detonation wave splits into two parts, a weak detonation which travels with the speed of one cell per time step and an ordinary shock wave.

We analyze a simplified set of equations and look for traveling wave solutions. It is shown that the solution depends on the dimensionless number $Kr = \frac{\mu K}{Q \rho_1}$. Here μ is the viscosity, K is the rate of reaction, Q is the heat release available in the process and ρ_1 is the density at the unburnt state. It is shown that the density peak of the traveling wave depends on Kr and also, that if Kr is sufficiently large there is no traveling wave solution. The erroneous behavior above is explained as an effect of the artificial viscosity necessarily inherent in the numerical methods when coarse grids are used. To prevent this unphysical behavior we suggest the use of an "artificial rate of reaction" such that the actual value of Kr used in the numerical method retains its correct physical value.

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2 Introduction

The last decade has seen rapid progress in high-resolution modeling of compressible gas dynamics. Using non-linear schemes developed in the last few years it is now possible to compute for example the interaction of shocks with other flow phenomena, and even strong embedded shocks can be treated without excessive numerical damping.

A particularly interesting phenomenon is the propagation of an exothermal chemical reaction by the thermodynamics of a compressible fluid. There are several propagation mechanisms, and that of primary interest here is a detonation wave, i.e. a compression shock wave which raises the temperature to initiate the reaction. To focus on the fluid mechanical part of the problem, one should select cases with simple and well established chemistry models. Even so, there are a large number of parameters, and charting out the whole space of reasonable parameter values is a formidable task. Here we will concentrate on some aspects of the phenomena to reduce the dimensionality of the parameter space.

The study of detonation waves has applications in for example modern air-breathing propulsion systems such as ram- and scram-jets for hypersonic vehicles and ram accelerators for projectiles, see [14, 7]. The pre-combustion compression necessary for a thermodynamically efficient propulsion is effected by a series of slanted stationary shock waves, and the ignition of the fuel-air mixture by a further shock. It is important to understand the dynamics of the ignition shock, which is not perfectly understood at present.

Such combustion phenomena are described by the Navier-Stokes equations for compressible fluid flow, with additional equations for the mass fractions of the different species. Many of the interesting phenomena observed in experiments can be obtained as the solution of these equations.

A simple model is obtained by assuming that the reaction takes place in a single step and that it can be modeled by only two or three species, unburnt (fuel+oxidant), burnt and possibly an inert diluant. We introduce the variable $Y(x,t)$ for the mass fraction of unburnt mixture under stoichiometric conditions. This leads to the following system

$$\rho_t + (\rho u)_x = 0 \tag{1}$$

$$(\rho u)_t + (\rho u^2 + p)_x - \mu u_{xx} = 0 \tag{2}$$

$$\rho(h + \frac{u^2}{2})_t + \rho u(h + \frac{u^2}{2})_x - p_t = (\lambda T_x)_x + \mu(uu_x)_x \tag{3}$$

$$(\rho Y)_t + (\rho u Y)_x = (\rho D Y_x)_x + \omega_a \tag{4}$$

Here μ is 4/3 times the dynamic viscosity, and the bulk viscosity is assumed to be zero. T is the temperature, ρ is the density, u is the mass average velocity, h is the enthalpy per unit mass, p is the pressure, D is the binary diffusivity and λ is the thermal conductivity. The term ω_a is the mass rate of production of mixture a. For a derivation of these equations see [14, 9].

To solve the extended Navier-Stokes system above we need:

1. A high-resolution numerical difference schemes for shock capturing, since the detonation waves are very steep.

2. A numerical solution procedure for the ordinary differential equations associated with the source term. Since ω_a is usually large (the time scales of the reactions are short) the method must be able to handle stiff ODE's.

It is well known that these requirements alone do not guarantee a satisfactory method. The coupling of the stiff ODE with the difference approximation sometimes leads to unphysical waves propagating with incorrect velocities, an effect which becomes more pronounced on coarse grids, see [13, 2]. This class of solution is commonly referred to as *spurious solutions*. In [4], Engquist and Sjögreen have suggested some remedies for this effect.

Here our approach is to analyze the underlying equations, not a specific numerical method. In particular, we want to investigate how the character of the solution depends on the physical parameters involved. It turns out that the occurrence of these spurious solutions can be explained as a side effect of the artificial viscosity, which is necessarily inherent in numerical methods when shock waves are present and the grid is coarse (or realistic). It is also follows that these solutions are physical in the sense that they exist when the product of the viscosity and the rate of reaction is large.

It is generally believed that in most cases a typical detonation consists of a very thin shock wave followed by a much thicker region where almost all the chemical reactions occur. This is the classical ZND theory, [14, 9]. This corresponds to the case when the scale of the shock wave is much smaller than the scale corresponding to the reaction, and can be considered as the limiting case when the viscosity tends to zero. In this article the behavior of the solution with varying ratio of these two scales is studied. This is a physical problem, but since it is difficult to find phenomena in nature where the scale of the shock wave is not small compared to the scale of the reaction it has its greatest importance in the context of numerical methods.

In [8] it is proposed that detonations cannot exist if the pressure is too large. This observation was probably due to numerical difficulties, since for large values of the ambient pressure the solution approaches the ZND detonation in such a way that the width of the shock wave is constant whereas the width of the reaction zone tends to infinity. The authors used a shooting method, starting in the vicinity of the burnt state. For large values of the ambient pressure (corresponding to small Kr, see notation below), this method becomes extremely sensitive to the initial, shooting data (this follows from an investigation of the behavior of the solution in the vicinity of the corresponding critical point), and it is easy to "run out of accuracy". This work is continued in [3], where an assumption of ignition kinetics is made. Here it is numerically verified that there exists a value of the rate of reaction above which no detonation is possible. This value corresponds to Kr_{cr} introduced below. For an investigation of the case when $Kr > Kr_{cr}$ we refer to [12].

In [15] the problem of slow reactions is considered. It is shown that a solution exists if the rate of reaction tends to zero. It is also shown that this solution approaches the

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ZND detonation, in the sense that the width of the shock wave is constant and the width of the reaction tends to infinity. Below it will be showed that the ZND detonation can be obtained by letting the viscosity approach zero while keeping the rate of reaction constant, in which case the thickness of the shock wave tends to zero and the thickness of the following deflagration stays constant. Considered in the phase space these two solutions are identical.

In [5] the existence of strong and weak detonation is proved under certain conditions on the diffusivity parameters involved (i.e. the viscosity, the heat conduction, and the species diffusion coefficient).

In [10] a *chord condition* is introduced, which if satisfied guarantees that no spurious solutions can occur. For our set of equations this condition would be satisfied if the ignition temperature is sufficiently high. This guarantees that a traveling wave solution exists independent of the viscosity or the rate of reaction, but a large value on the artificial viscosity will change the solution drastically, for instance the pressure peak will be lost (so in that sense this solution might still be called spurious).

Previously we have studied a simplified problem, essentially Burgers equation with a source term mimicking the chemistry, [11]

$$u_t + g(u)u_x = -Kf(u) + \nu u_{xx}. \tag{5}$$

The stiffness of this problem can be varied by changing the factor K (corresponding to the rate of reaction) in the source term. It was found that traveling wave solutions exist which look physically reasonable but move with an incorrect propagation speed if an artificial viscosity is used. This erroneous behavior becomes more and more pronounced when the stiffness of the problem is increased. The speed of the wave depends on the viscosity ν and the rate of reaction K in the combination νK. When this product is large the speed of the wave is proportional to $\sqrt{\nu K}$. This agrees with the result of the classical Thermal theory, see [14, 9]. On the other hand, for small values of this product the speed of the wave is almost constant, independent of νK.

The result above suggests the investigation of the full 1-D Navier-Stokes equations with a single reaction, Eqs.(1-4). It will be shown that the conclusions drawn from the simpler model above can be verified if we make the simplifications $\lambda = D = 0$ (i.e. we neglect the heat conduction and the diffusion of the two mixtures) and use Heaviside kinetics

$$\omega_a = -KH(T - T_i)\rho Y. \tag{6}$$

Here K is again the rate of reaction, H is the Heaviside function and T_i is the ignition temperature. The assumption of Heaviside kinetics is made in order to avoid the *cold boundary difficulty*, see [14, 9]. Apart from these assumptions it is also assumed that the specific heats at constant pressure of the two mixtures involved are constant and equal. Further we assume that μ is constant and that the molecular masses of the two mixtures are equal.

We introduce the dimensionless number $Kr = \frac{\mu K}{Q\rho_1}$ where Q is the difference in heat of formation of the two mixtures and ρ_1 is the value of ρ on the cold side of the

detonation. If we assume that the initial and final states are chosen so that a strong detonation wave is possible then we can show that there exists a unique $Kr = Kr_{cr}$ such that if

- $Kr < Kr_{cr}$ a traveling wave solution exists between the initial and final state. Here the speed is uniquely determined by these states. In this case a density peak is possible, i.e. the maximum value of the density is higher than the value at the final state. This solution is a strong detonation.

- $Kr \geq Kr_{cr}$ no traveling wave solution exists between the given states.

If it is instead assumed that the states are given in such a way that a Chapman-Jouget detonation wave is admissible, the existence of a unique $Kr = Kr_{cr}$ can be shown such that if

- $Kr < Kr_{cr}$ a traveling wave solution exists between the given states, the speed is uniquely determined by these states. In this case the density profile has to have a density peak.

- $Kr = Kr_{cr}$ the situation is the same as above except that for this case the density profile is monotone.

- $Kr > Kr_{cr}$ no traveling wave solution exists between the given states.

For a definition of strong and Chapman-Jouget detonations see [14, 9].

The conclusion here is that it is important to keep Kr at its correct physical value when solving Eqs.(1-4) numerically. This conclusion suggests the following general way of modifying current numerical schemes: If an artificial viscosity, $\mu + \mu_a > \mu$, is inherent in the numerical method, use also an "artificial rate of reaction", K_a, such that $(\mu + \mu_a)K_a = \mu K$ and Kr retains its correct value. By this action the shock will wider, but the amount of reactions taking place over it will be correct. If it is further assumed that $\mu_a = c\Delta x \ll \mu$ it follows that the artificial rate of reaction is equal to $(1 - \frac{c}{\mu}\Delta x + O(\Delta x^2))K$, i.e. the method is first order accurate (even though it is slightly dubious to talk about order of accuracy in this case since if $\mu_a = c\Delta x \ll \mu$ the shock wave is resolved and the artificial viscosity is superfluous). The solution corresponding to the inviscid equations is a ZND detonation and in order to obtain it numerically the reaction should be switched off entirely in the interior of the shock wave. For work along these lines see [4].

One should not use an artificial ρ_1 since that would alter the initial state. For similar reasons Q cannot be changed.

3 Analysis

In the appendix, based on the Navier-Stokes equations and certain assumptions, the equations to be used here are derived. In short the following is assumed:

- the heat flux and the diffusion of species are neglected,

- the *law of mass action* holds,

- Heaviside kinetics is adequate,

- only two species are involved in the reaction (+ possibly an inert diluant),

- the specific heats are equal and constant,

- the molecular masses are the same,

- a traveling wave solution exists.

The equations are written in nondimensional form, and it turns out that in this context the dimensionless number $\frac{\mu K}{Q \rho_1}$ is important. Here μ is the dynamic viscosity, Q is the difference in heat of formation of the two species involved in the reaction, K is the rate of reaction and ρ_1 is the density at the unburnt state. Henceforth this dimensionless number is denoted by Kr - the *Kreiss number*.

As a result of the assumptions above the following two differential equations

$$v' = \frac{1}{sv}(\gamma - 1)(p(v; s^2) - Y), \tag{7}$$

$$Y' = -Kr H(T - T_i) \frac{1}{sv} Y, \tag{8}$$

and the algebraic relation

$$T = \gamma(q(v; s^2) - Y) + T_i \tag{9}$$

emerge. Here v is the specific volume, Y is the mass fraction of unburnt gas and T is the temperature. Furthermore, s is the speed of the traveling wave, T_i is the ignition temperature and $\gamma = C_p/C_v$. $p(v; s^2)$ and $q(v; s^2)$ are quadratic expressions in v. The Heaviside kinetics is described by the function $H(T - T_i)$. All the variables here are in nondimensional form. For details see the appendix.

In what follows the subindex i is used to denote the variables at the point of ignition and the subindex 1 specifies the variables at the initial state ($v_1 = 1$ since this variable has been normalized with the value of the specific volume at the initial state).

The purpose in this section is to find a solution curve (or phase curve) which connects the initial state with some possible final state. The solution will be sought for in the phase space - in this case R^2, with coordinates denoted by (v, Y) in accordance with Eq.(7,8) above. The initial and final states have to be critical points (i.e. points in the phase plane where $v' = Y' = 0$). In section 3.1 below it is shown under which conditions these critical points exist, and in section 3.2 the behavior of the solution curves in their vicinity is described. In section 3.3 the question of existence of a solution curve connecting the initial and the final states is addressed. The significance of Kr is also discussed here. In section 3.4 it is shown that as the viscosity tends to zero the so called ZND-detonation is obtained.

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Denote by $S(z)$ the solution of Eqs.(7,8). Note that if $S(z)$ is a solution then so is $S(z + \Delta)$, ($\Delta =$ constant). These solutions are considered identical. In order to get rid of this ambiguity $S(z)$ is fixed at some specific z, choose z_i to be the z-value at the point of ignition. I.e., $S(z) = (v(z), Y(z))$ and $S(z_i) = (v_i, Y_1)$.

It is obvious from Eqs.(7,8) that if $S(z) = S_1(z)$ is a solution for $s = s_1 > 0$ then $S(z) = S_1(-z)$ is a solution for $s = -s_1$. Therefore, in what follows, only non-negative s will be considered (corresponding to a wave traveling to the left).

3.1 Critical Points

At the initial and the final state both v' and Y' have to be zero. From Eqs.(7,8) it is seen that:

- $v' = 0$ whenever $Y = p(v; s^2)$, and

- $Y' = 0$ when $T < T_i$ (and $H(T - T_i) = 0$) or when $Y = 0$. From Eq.(9) it follows that $T < T_i$ whenever $Y > q(v; s^2)$.

In a detonation the mixture is ignited by the rise in temperature due to a strong compression. Hence, at the initial state T has to be less than T_i, therefore Y has to be larger than $q(v; s)$ there. In general, for those domains in the phase plane where $Y > q(v; s^2)$ the solution curves are straight lines parallel to the v-axis, and these solution curves are parts of ordinary shock waves without any combustion. At the final state on the other hand the reaction should be finished and it has to be required that $Y = 0$. Hence, in order for a detonating wave to exist the following has to hold at the critical points involved:

- $Y > q(v; s^2)$ and $Y = p(v; s^2)$ at the initial state, and

- $Y = 0$ and $Y = p(v; s^2)$ at the final state.

It will next be shown that for sufficiently large values on s, critical points exists which satisfies these requirements.

The expression for $p(v; r)$, Eq.(95), can be written

$$p(v; r) = \frac{1}{2}\frac{\gamma + 1}{\gamma - 1}(v - \frac{\gamma - 1}{\gamma + 1})(v - 1)r - T_1(v - 1) + Y_1 \tag{10}$$

where $r = s^2$ has been introduced (T_1 and Y_1 are the values of T and Y at the initial state). From this equation it follows that:

- For all $r > 0$ the curve $Y = p(v; r)$ is a parabola which has to pass through the points

$$(a_1, b_1) \text{ and } (1, Y_1) \text{ where } a_1 = \frac{\gamma - 1}{\gamma + 1} \text{ and } b_1 = \frac{2}{\gamma + 1}T_1 + Y_1. \tag{11}$$

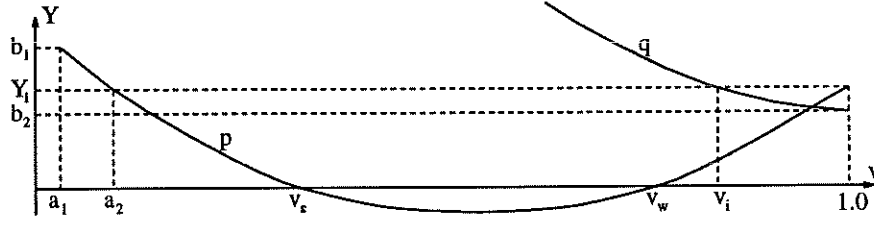Here it is noted that $a_1 > 0$ and that $b_1 > Y_1$, see Fig. 1.

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Figure 1: qualitative picture for relevant values on s and T_i

- If $r = 0$ the curve $Y = p(v; r)$ is a straight line intersecting the v-axis at $v = 1 + \frac{Y_1}{T_1}$.

- If $v \in (a_1, 1)$ then $p(v; r)$ can be made arbitrarily small by increasing r.

Hence, for sufficiently large r the parabola $Y = p(v; r)$ has two zeroes which both belong to the interval $(a_1, 1)$. For a qualitative picture of the curve $Y = p(v; s)$ see Fig. 1.

As stated above, a detonation is characterized by a strong compression and since $v = 1$ at the initial state it has to be required that $v < 1$ at the final state. Therefore, a detonation is only possible for large r. It can be shown that $r \geq r_b$, where

$$r_b = \left((\gamma + 1)Y_1 + T_1 + \sqrt{((\gamma + 1)Y_1 + 2T_1)(\gamma + 1)Y_1} \right) (\gamma - 1) \qquad (12)$$

is the condition which has to be satisfied. Henceforth only $r \geq r_b$ is considered. With this choice of r it is obvious that $a_2 > 0$. Here a_2 is the value of $v < 1$ at the intersection between $Y = Y_1$ and $Y = p(v; s^2)$. This guarantees that the minimum value of v is always larger than zero ($v \geq a_2 > 0$).

If $r > r_b$ then two possible final states exist. These are denoted by $(v_s, 0)$ and $(v_w, 0)$, see Fig. 1. The detonation is called strong if it ends up at $(v_s, 0)$ and weak if it ends up at $(v_w, 0)$. If on the other hand $r = r_b$ only one possible final state exists, and in this case the solution ending up at this critical point is called a Chapman-Jouget detonation.

The critical point specifying the initial state is given by $(1, Y_1)$. The point of ignition, denoted by (v_i, Y_1) are defined by the intersection of the line $Y = Y_1$ and the curve $Y = q(v; s^2)$ (to the left of $v = 1$). The following is required:

- The critical point specifying the initial state has to lie above the curve $Y = q(v; s^2)$ (this is follows since Y' should be zero at that point). This implies that $v_i < 1$.

- $v_i > v_w$, this is required since it is more adequate from physical considerations, and since the behavior of the solution is quite different if this is not satisfied. It turns out that if this is not fulfilled the weak detonation solution is ruled out, and also that a traveling wave solution exists independently of Kr.

Eq.(96) shows that $Y = q(v; r)$ is a convex parabola passing through the point $(1, b_2)$, where $b_2 = \frac{1}{\gamma}(T_1 - T_i) + Y_1$ for all values on r. It also holds that the minimum of this

curve occurs for $v > 1$ independent of r. It follows that it is always possible to choose T_i in such a way that the requirements above are fulfilled.

With the above assumption on r and T_i, which will be kept throughout the paper, the situation is qualitatively as depicted in Fig. 1.

3.2 Final States

From section 3.1 it is clear that the possible values of v at the final states are given by

$$p(v; s^2) = 0. \tag{13}$$

This yields

$$v_{0,2} = \frac{\gamma s^2 + (\gamma - 1)T_1}{s^2(\gamma + 1)} \mp \frac{\sqrt{(\gamma s^2 + (\gamma - 1)T_1)^2 - 2s^2(\gamma + 1)(\gamma - 1)(\frac{1}{2}s^2 + T_1 + Y_1)}}{s^2(\gamma + 1)}. \tag{14}$$

If $s^2 > r_b$ these two roots are distinct and satisfy $a_1 < v_s < v_w < 1$. If this is the case the solution of the complete, non-linear equations behave in the same way in a sufficiently small neighborhood around the critical points. If on the other hand $s^2 = r_b$ only one critical point exists. In this case the linearized equations can not be used to determine the behavior of the solution of the non-linear equations. Therefore only the case $s^2 > r_b$ is considered in the linear analysis below.

For future reference $p(v, s^2)$ is rewritten as

$$p(v; s^2) = \frac{1}{2}s^2\frac{\gamma + 1}{\gamma - 1}(v - v_s)(v - v_w). \tag{15}$$

With the choice of s being positive, the unburnt state is approached as $z \to -\infty$ and the burnt state is approached as $z \to \infty$. Therefore, when considering the solution curves approaching the final states, only the stable manifolds are of interest (the set of solutions curves approaching the final states with increasing z).

Below it is demonstrated that the character of the solution corresponding to the linearized equations are completely different for the strong and the weak detonation. It is also shown that the character of the solution is greatly dependent of Kr in the vicinity of $(v_s, 0)$.

3.2.1 Linearization Around v_s

Make the ansatz

$$v = v_s + x_1 \tag{16}$$

$$Y = 0 + x_2. \tag{17}$$

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It has already been assumed that $T > T_i$ in a neighborhood of $(v_s, 0)$, and consequently $H(T - T_i) = 1$ there (otherwise no detonation is possible). If quadratic and higher order terms are neglected substitution of this in Eq.(7) and Eq.(8) yield

$$\left(\begin{array}{c} x_1 \\ x_2 \end{array} \right)' = A \left(\begin{array}{c} x_1 \\ x_2 \end{array} \right) \tag{18}$$

where

$$A = \left(\begin{array}{cc} d_1 & -\kappa \\ 0 & d_2 \end{array} \right) \tag{19}$$

with

$$d_1 = \frac{1}{sv_s}(\gamma - 1)p'(v_s; s^2), \quad \kappa = \frac{1}{sv_s}(\gamma - 1) \text{ and } d_2 = -\frac{Kr}{sv_s}. \tag{20}$$

d_1 and d_2 are the eigenvalues of the matrix A. Since only positive s are considered it follows that d_1 and d_2 are both negative. The general solution of Eq.(18) with $x_1 = x_1(z_0)$ and $x_2 = x_2(z_0)$ at $z = z_0$ (since the system is autonomous z_0 is arbitrary) are

$$x_1 = x_1(z_0)e^{d_1(z-z_0)} - \frac{\kappa x_2(z_0)}{d_2 - d_1}(e^{d_2(z-z_0)} - e^{d_1(z-z_0)}) \tag{21}$$

$$x_2 = x_2(z_0)e^{d_2(z-z_0)} \tag{22}$$

$$\text{when } d_1 \neq d_2 \text{ or,} \tag{23}$$

$$x_1 = x_1(z_0)e^{d_1(z-z_0)} - \kappa x_2(z_0)e^{d_1(z-z_0)}(z - z_0) \tag{24}$$

$$x_2 = x_2(z_0)e^{d_1(z-z_0)} \tag{25}$$

$$\text{if } d_1 = d_2. \tag{26}$$

I.e. improper, stable nodes in both cases, see [1] (this means that every solution curve tends to the origin as $z \to \infty$, and that every solution curve, except one when $d_1 \neq d_2$, has the same limiting direction there). Only $x_2(z_0) > 0$ is considered here since $x_2(z_0) = 0$ would imply $x_2 \equiv Y \equiv 0$ corresponding to an ordinary shock wave without any combustion.

Since $x_2(z_0) \neq 0$ the quotient $x_1/x_2 = (v - v_s)/Y$ can be used to explain the behavior of the solution as the critical point is approached. If $d_1 \neq d_2$ then

$$\frac{x_1}{x_2} = \left(\frac{x_1(z_0)}{x_2(z_0)} + \frac{\kappa}{d_2 - d_1}\right)e^{(d_1 - d_2)(z - z_0)} - \frac{\kappa}{d_2 - d_1}. \tag{27}$$

Otherwise

$$\frac{x_1}{x_2} = \frac{x_1(z_0)}{x_2(z_0)} - \kappa(z - z_0). \tag{28}$$

These formulas imply that the behavior as $z \to \infty$ depends on the relationship between d_1 and d_2. One can distinguish between the following three cases:
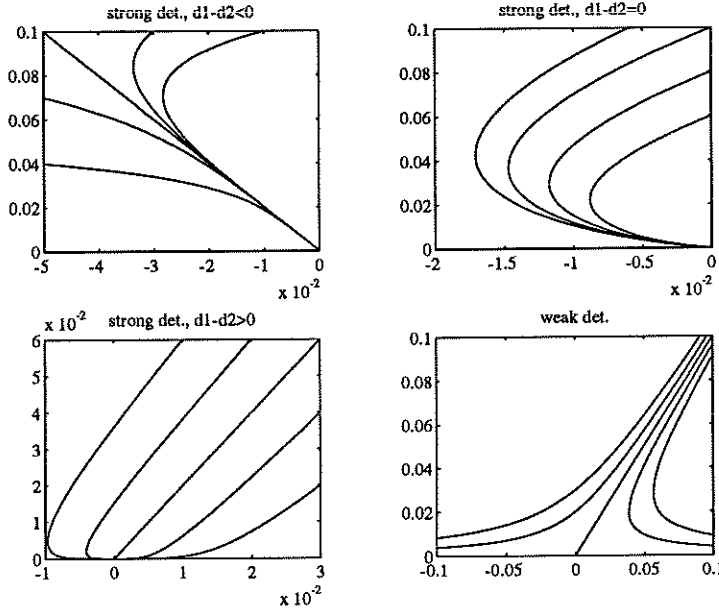
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Figure 2: the linearized solution around the weak and strong detonation states

- If $d_1 - d_2 < 0$, i.e. Kr "small" then

$$\lim_{z \to \infty} \frac{x_1}{x_2} = \frac{\kappa}{d_1 - d_2} = \frac{\gamma - 1}{(\gamma - 1)p'(v_s; s^2) + Kr} < 0, \qquad (29)$$

see Fig. 2. It follows that there has to be a density peak (since $\rho = 1/v$).

- If $d_1 = d_2$ then

$$\lim_{z \to \infty} \frac{x_1}{x_2} = \lim_{z \to \infty} (-\kappa z) = \infty \qquad (30)$$

and there is a density peak in this case also, but the character is different from the case above, see Fig. 2.

- If $d_1 - d_2 > 0$, i.e. Kr "large" then

$$\lim_{z \to \infty} \frac{x_1}{x_2} = \pm \infty \qquad (31)$$

for all solution curves except when $\frac{x_1(z_0)}{x_2(z_0)} = \frac{\kappa}{d_1 - d_2}$, see Fig. 2. Hence the linearized analysis does not guarantee the existence of a density peak as it did in the two previous cases.

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The complete equations in the new variables become

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}' = A \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \tag{32}$$

where

$$f_1 = \frac{\gamma - 1}{s} \frac{(p''(v_s; s^2)v_s - 2p'(v_s; s^2))x_1^2 + 2x_1 x_2}{2v_s(v_s + x_1)} \text{ and } f_2 = \frac{Kr}{s} \frac{x_1 x_2}{v_s(v_s + x_1)}. \tag{33}$$

The fact A have no eigenvalues with zero real part, together with the fact that both f_1 and f_2 tend to zero as $O(x_1^2 + x_2^2)$ (as the origin is approached) and have continuous derivatives show that the solution of the complete equations behave in the same way as the solution of the linearized equations near the origin, see [1].

3.2.2 Linearization Around v_w

Linearization around $(v_w, 0)$ yields the same equations as above, but in this case

$$d_1 = \frac{1}{sv_w}(\gamma - 1)p'(v_w; s^2), \; \kappa = \frac{1}{sv_w}(\gamma - 1) \text{ and } d_2 = -\frac{Kr}{sv_w}. \tag{34}$$

d_1 is positive. Hence, the eigenvalues of A are of different sign and $(v_w, 0)$ is a saddle point. In order for the solution to stay bounded as $z \to \infty$, Eq.(21) shows that it has to be required that

$$\frac{x_1(z_0)}{x_2(z_0)} = \frac{\kappa}{d_1 - d_2}. \tag{35}$$

Therefore, only for those values on $x_1(z_0)$ and $x_2(z_0)$ which satisfy the above equation will the solution of the linearized equation stay bounded. Eq.(35) also specifies the direction of the stable manifold at the saddle point $(v_w, 0)$ - which in this case consists of just one solution curve, see Fig. 2.

In the same way as above it can shown that the solution of the complete equations behave in the same way as the solution of the linearized equations.

3.3 Existence of a Solution

As stated earlier it is assumed that $s \geq \sqrt{r_b}$ and that T_i is chosen such that $v_i > v_w$. The case when $s > \sqrt{r_b}$, the strong and the weak detonation, is treated in detail in section 3.3.1, and in section 3.3.2 the result concerning the Chapman-Jouget detonation is presented.
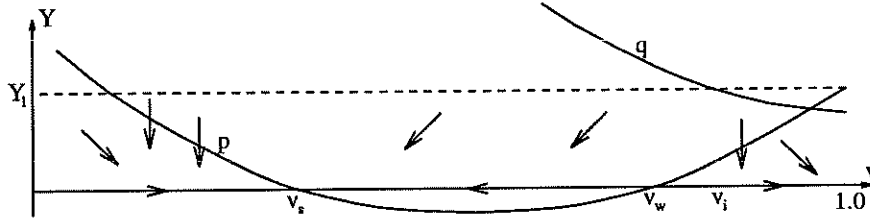
Figure 3: the slopes of the solution curves

3.3.1 Strong and Weak Detonations

For further reference the following can be noted about the solution curves:

- $v' < 0$ above the curve $Y = p(v; s^2)$ and $v' > 0$ below it.

- $Y' < 0$ between the curves $Y = q(v; s^2)$ and $Y = 0$.

For the slope of the solution curves below the curve $Y = q(v; s^2)$ (i.e. when $T > T_i$) Eqs.(7,8) yield:

$$\frac{Y'}{v'} = Kr \frac{Y}{M(v, Y; s^2)} \tag{36}$$

where

$$M(v, Y; s^2) = (\gamma - 1)(Y - p(v; s^2)). \tag{37}$$

From Eq.(8) it follows that every point of the v-axis is part of a solution curve never leaving the same axis. Eq.(7) indicates that every solution curve crossing the curve $Y = p(v; s^2)$, below $Y = q(v; s^2)$, is parallel to the Y-axis at the point of intersection. From these two equations it also follows that every solution curve above the curve $Y = p(v; s^2)$ is directed to the left, whereas those below are directed to the right. In Fig. 3 these facts are schematically demonstrated.

The Heaviside function in Eq.(8) suggests that $S(z)$ is split in two parts. The first part is the straight line $Y = Y_1$ connecting the initial state $(1, Y_1)$ with (v_i, Y_1). The second part of the solution connects (v_i, Y_1) with one of the two possible final states, $(v_s, 0)$ or $(v_w, 0)$.

With the assumption on T_i above the following theorem can be proved:

Theorem 1 *If $s > \sqrt{T_b}$ there exists a unique $Kr = Kr_{cr}$ such that*

- *For $Kr < Kr_{cr}$ there exists a unique solution connecting the initial state with the final state $(v_s, 0)$. This is a strong detonation.*

- *For $Kr = Kr_{cr}$ there exists a unique, monotonic solution connecting the initial state with the final state $(v_w, 0)$. This is a weak detonation.*
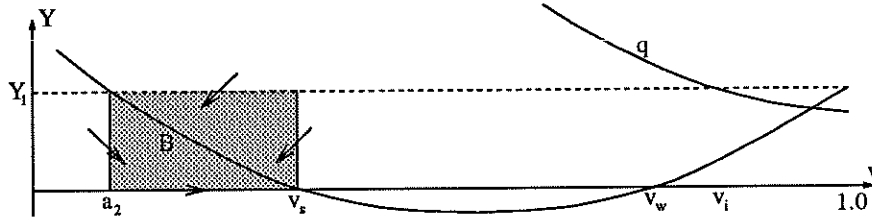
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Figure 4: arrows indicate directions of solution curves for increasing z

- *For $Kr > Kr_{cr}$ no solution exists connecting the initial state with either of the two possible final states.*

Lemmas 1-4 below are used to prove this theorem.

Lemma 1 *If Kr is sufficiently small then there exists a unique solution, connecting the initial state with the final state $(v_s, 0)$.*

Proof: Eq.(36) shows that by choosing Kr sufficiently small the solution curve emerging from (v_i, Y_1) has to enter the region B bounded by the curves $v = a_2$, $Y = 0$, $v = v_s$ and $Y = Y_1$, see Fig. 4.

   B can be considered as a closed subset of D, where D is a bounded open subset of the (v, Y) plane which contains only a finite number of critical points (only one). It also holds that on the boundary of B no solution curves are directed out of B. Specifically the v-axis is a solution curve, and uniqueness considerations prevents any solution curve containing points with $Y > 0$ to cross that axis. From a theorem concerning autonomous systems it follows that the only possibility for solution curves which has entered B is to approach $(0, v_s)$ as $z \to \infty$, see [1].

●

Lemma 2 *No solution exists between the initial state and any of the two possible final states for Kr sufficiently large.*

Proof: In the same way as for the lemma above it can be shown that for sufficiently large Kr the solution curves leaving the point of ignition has to cross $Y = p(v; s^2)$ with $v \in (v_w, v_i)$. Further, below $Y = p(v; s^2)$ the velocity field is directed to the right and there is no possibility for any solution curve to reach either $(v_s, 0)$ or $(v_w, 0)$ as $z \to \infty$.

●

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Lemma 3 *Solution curves emerging from* (v_i, Y_1) *for different Kr can only intersect each other below the curve $Y = p$ or at the point $(v_s, 0)$.*

Proof: Consider the second part of the solution, i.e. the part where $T \geq T_i$. For this solution $Y' < 0$ as long as $Y > 0$ (as noted before $Y = 0$ can only be attained at the critical points $(v_s, 0)$ or $(v_w, 0)$). Hence the inverse of $Y(z)$ exists, denote it by h (i.e. $z = h(Y)$). If φ is defined by $\varphi(Y) = v(h(Y))$ it satisfies the equation

$$\frac{d\varphi}{dY} = \frac{\gamma - 1}{Kr} \frac{Y - p(\varphi)}{Y} \text{ with } \varphi(Y_1) = v_i. \tag{38}$$

Let φ_1 and φ_2 denote the solutions with $Kr = Kr_1$ and $Kr = Kr_2$ respectively. Without loss of generality it can be assumed that $Kr_1 < Kr_2$. Define Ψ by $\Psi = \varphi_2 - \varphi_1$. Hence

$$\frac{d\Psi}{dY} = \frac{\gamma - 1}{Kr_1 Kr_2} \left(Kr_1 \frac{Y - p(\varphi_2)}{Y} - Kr_2 \frac{Y - p(\varphi_1)}{Y} \right). \tag{39}$$

Since $\frac{d\Psi(Y_1)}{dY} < 0$ it follows that there exists a τ such that $\Psi(Y) > 0$ for $\tau < Y < Y_1$.

The following assumptions are now made:

- φ_1 and φ_2 intersect each other above or on the curve $Y = p(v; s^2)$ with a value of $Y > 0$.

- φ_1 and φ_2 end up at the saddle point $(v_w, 0)$.

For both cases it is shown that these assumptions lead to contradictions.

For the first case, let $\mu = \inf \tau$. From continuity $\Psi(\mu) = 0$. Eq.(15) is used to rewrite the expression for $p(\varphi_2)$

$$p(\varphi_2) = p(\varphi_1) + \alpha \left(\Psi(2\varphi_1 - (v_s + v_w)) + \Psi^2 \right) \text{ where } \alpha = \frac{1}{2} s^2 \frac{\gamma + 1}{\gamma - 1} \tag{40}$$

and hence

$$\frac{d\Psi}{dY} = \frac{\gamma - 1}{Kr_1 Kr_2} \left((Kr_1 - Kr_2) \frac{Y - p(\varphi_1)}{Y} - Kr_1 \alpha \frac{\Psi(2\varphi_1 - (v_s + v_w)) + \Psi^2}{Y} \right). \tag{41}$$

If the two solution curves intersect above the curve $Y = p(v; s^2)$ it immediately follows that $\frac{d\Psi(\mu)}{dY} < 0$ and therefore $\Psi(\mu + \varepsilon) < 0$ for small ε. This is a contradiction to the fact that $\Psi(Y) > 0$ for $\mu < Y < Y_1$. If on the other hand the solution curves intersect on the curve $Y = p(v; s^2)$ a constant k can be found such that the following holds

$$\frac{d\Psi}{dY} \leq k\Psi \tag{42}$$

where either

$$k > \alpha \frac{\gamma - 1}{Kr_2} \frac{v_w - v_s}{\mu} \text{ or } k < -\alpha \frac{\gamma - 1}{Kr_2} \frac{v_w - v_s}{\mu}. \tag{43}$$
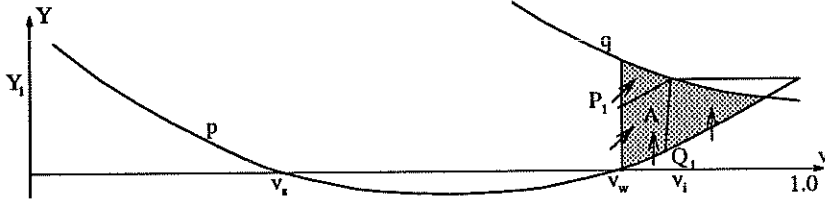
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Figure 5: arrows indicate directions of solution for decreasing z

Therefore Ψ is identically zero in a neighborhood of $Y = \mu$ which is again a contradiction.

For the second case the linearized analysis and the result above show that a contradiction is reached. In a neighborhood of the saddle point

$$\Psi(Y) = \left((\gamma - 1)\frac{Kr_1 - Kr_2}{((\gamma - 1)p'(v_w; s^2) + Kr_1)((\gamma - 1)p'(v_w; s^2) + Kr_2)}\right) Y + O(Y^2) \quad (44)$$

and therefore $\Psi(Y) < 0$ for sufficiently small Y.

●

Lemma 4 *There exists a unique $Kr = Kr_{cr}$ which gives a unique, monotonic solution between the initial state and the final state $(v_w, 0)$, see Fig. 5.*

Proof: Let A be the region bounded by the curves $Y = q(v; s^2)$, $v = v_w$ and $Y = p(v; s^2)$, see Fig. 5. From lemma 1 and 2 it follows that Kr_{p1} and Kr_{q1} exist such that $0 < Kr_{p1} < Kr_{q1} < \infty$ and such that $S(z; Kr_{p1})$ leaves A somewhere on $v = v_w$ and $S(z; Kr_{q1})$ leaves A on $Y = p(v; s^2)$. Denote these points of intersections by P_1 and Q_1 respectively, and let d_1 be the minimum value of Y of these two points.

Next, let P_2 and Q_2 be points on $v = v_w$ and $Y = p(v; s^2)$ with a value of Y equal to d_2, where $d_2 = d_1/2$. Consider solution curves from these two points with *decreasing* z, and denote them by $L(z; P_2, Kr)$ and $L(z; Q_2, Kr)$.

Any solution curve in A can only leave the region through the curve $Y = q(v; s^2)$ as z decreases. On the other two boundaries all solution curves are directed towards the interior (for decreasing z). Further, except for points with a distance less than ε away from the curve $Y = p(v, s^2)$ the slopes of the solution curves in A can be bounded by

$$Kr K_1 \leq \frac{Y'}{v'} \leq Kr K_2, \text{ where } 0 < K_1 < K_2 < \infty. \quad (45)$$

For points within a distance ε from the curve $Y = p(v; s^2)$
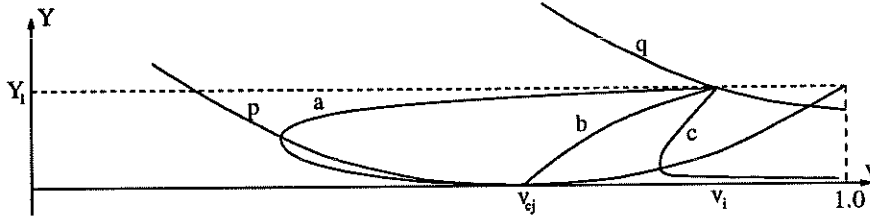
$$Kr K_2 \leq \frac{Y'}{v'} \quad (46)$$

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Figure 6: solution curves for different values on Kr

holds for the slope of the solution curves. Since T_i has been chosen such that $v_w < v_i < 1$, and since ε above is arbitrary it follows that by choosing Kr large enough $L(z; P_2, Kr)$ will eventually reach $Y = q(v; s^2)$ to the left of the point (v_i, Y_1) as z decreases. Similarly, by choosing Kr small enough $L(z; P_2, Kr)$ will eventually leave A to the right of the point of ignition. The same is true for $L(z; Q_2, Kr)$. From continuity considerations, and from lemma 3 it then follows that unique Kr_{p2} and Kr_{q2} can be found such that $Kr_{p1} < Kr_{p2} < Kr_{q2} < Kr_{q1}$ and that both $L(z; P_2, Kr_{p2})$ and $L(z; Q_2, Kr_{q2})$ passes through the ignition point (v_i, Y_1).

This process can be continued indefinitely toward $(v_w, 0)$ and therefore a Kr_{cr} exists such that a $S(z; Kr_{cr})$ exists which tends to $(v_w, 0)$ as $z \to \infty$.

Uniqueness of Kr_{cr} is guaranteed by lemma 3. Non uniqueness would be a contradiction of that lemma. From the linearization it is further known that $S(z; Kr_{cr})$ is unique.

•

3.3.2 Chapman-Jouget Detonation

In this case $s^2 = r_b$ and only one critical point is possible, $(v_{cj}, 0)$, see Fig. 6. For this situation the following can be proved

Theorem 2 *If* $s = \sqrt{r_b}$ *there exists a unique* $Kr = Kr_{cr}$ *such that*

- *For* $Kr < Kr_{cr}$ *there exists a unique solution connecting the initial state with the final state* $(v_{cj}, 0)$, *and approaching the critical point below the curve* $Y = p(v; s^2)$, *curve a in Fig. 6.*

- *For* $Kr = Kr_{cr}$ *there exists a unique, monotonic solution connecting the initial state with the final state* $(v_{cj}, 0)$, *curve b in Fig. 6.*

- *For* $Kr > Kr_{cr}$ *no solution exists connecting the initial state with the final state* $(v_{cj}, 0)$, *curve c in Fig. 6.*

Except for obvious modifications in notations lemma 1 and 2 are still valid. Lemma 4 can still be used to prove the existence of a Kr_{cr} for which a monotonic solution
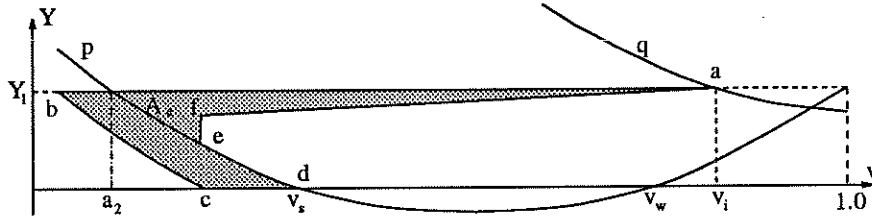
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Figure 7: the solution curves must stay in A_e

exists. In order to show uniqueness of Kr_{cr} lemma 3 can be used but the proof has to be modified since in this case the linearized analysis can not be used in the vicinity of the critical point. For the same reason the uniqueness of the solution has to be proved in a different way. These extensions will be carried out in the appendix.

3.4 The ZND detonation

A ZND detonation is a detonation which consists of a shock wave with no combustion followed by a much thicker region where the chemical reaction occurs, a deflagration, see [14, 9]. In this section the following is proved

Theorem 3 *As $\mu \to 0$ the solution of Eqs.(7,8) tends to a ZND-detonation.*

Proof: Consider the closed subset A_e in Fig. 7. The coordinates of the corners of A_e are: $a = (v_i, Y_1)$, $b = (a_2 - \varepsilon, Y_1)$, $c = (v_s - \varepsilon, 0)$, $d = (v_s, 0)$, $e = (a_2 + \varepsilon, Y_e)$ and $f = (a_2 + \varepsilon, Y_1 + \frac{k}{2}\varepsilon)$. Here $\varepsilon > 0$, $k = \frac{dp(a_2)}{dv}$ and Y_e is the the value of Y at the intersection between the vertical line through f and $Y = p(v, s^2)$. It will be shown that on the boundaries of A_e no solution curves are directed out of A_e for sufficiently small Kr and the solution has to be contained in A_e. Therefore if the solution enters this closed subset it has to approach the critical point $(v_s, 0)$ as $z \to \infty$, see [1].

- On the line between a and b it holds that $Y' < 0$ for all $Kr > 0$ and hence all solution curves are directed into A_e.

- On the curve between b and c Eq.(36) shows that for sufficiently small Kr all solution curves are directed inwards (the curve between b and c is constructed so that its slope everywhere is less than 0).

- The line between c and d is a solution curve and it is impossible for an other solution curve to cross this line by uniqueness.

- On the curve between d and e it holds that $v' = 0$ and $Y' \leq 0$ and it is again impossible for a solution curve to leave A_e through this part of the boundary.

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- On the line between e and f it is noted that $v' \leq 0$ and no integral curve can leave A_e through this line.

- Finally, Eq.(36) again shows that all integral curves on the line between f and a are directed to the interior of A_e for sufficiently small Kr. In the same way it holds that for sufficiently small Kr the integral curve emerging from (v_i, Y_1) is directed into A_e (this point is not a critical point).

From the scaling in Eq.(56) it follows that the thickness of the shock is $O(\mu)$.

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4 Conclusion

For a simplified set of equations we have been able to explain the difficulties encountered when detonations are treated numerically. It has been shown that an important physical parameter in this context is the product between the viscosity and the rate of reaction. The traveling wave solution of this set of equations is gradually changed as this product is increased from a small value – typically the peak value of the density is lowered – and for sufficiently large values the traveling wave solution ceases to exist. Therefore, in numerical treatment of detonation problems, it is suggested that the reaction rate is modified in such a way that the product of itself and the artificial viscosity used in the numerical method is identical to its correct physical value (if the fluid flow problem under consideration is inviscid it is suggested that the reactions are totally switched off in the interior of the shock wave).

5 Acknowledgment

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A   Derivation of Equations

It is assumed that the combustion process can be represented by a single one step reaction involving only two or three species, unburnt with index a (fuel+oxidant) and

burnt gas with index b (product) and possibly an inert diluant. The standard equations take the following form

$$\rho_t + (\rho u)_x = 0, \tag{47}$$

$$(\rho u)_t + (\rho u^2 + p)_x - \mu u_{xx} = 0, \tag{48}$$

$$\rho(h + \frac{u^2}{2})_t + \rho u(h + \frac{u^2}{2})_x - p_t = -q_x + \mu(u u_x)_x, \tag{49}$$

$$(\rho Y)_t + (\rho u Y)_x = (\rho D Y_x)_x + \omega_a. \tag{50}$$

As usual, ρ, u and h represents the density ($\rho = \rho_a + \rho_b$), mass-average velocity ($u = (\rho_a u_a + \rho_b u_b)/\rho$) and the enthalpy per unit mass ($h = h_a Y + h_b Z$). Y is the mass fraction of unburnt gas ($Y = \rho_a/\rho$) and Z is the mass fraction of burnt gas. p is the pressure ($p = p_a + p_b$) and q is the heat flux. The constant μ represents viscosity ($\mu = 4/3$ times the dynamic viscosity, and here the bulk viscosity has been assumed to be zero). D is the binary diffusivity. The term ω_a is the mass rate of production of mixture a (the unburnt mixture). For the derivation of these equations see [14, 9].

In this section a traveling wave ansatz will be made. The equations will also be simplified in order to get them in a form suitable for the analysis in the subsequent sections.

It is assumed that

$$\omega_a = -K k(T) \rho Y \tag{51}$$

and that $q_x = (\rho D Y_x)_x = 0$, i.e. the heat flux and the diffusion of species are neglected. To describe ω_a the *law of mass action* has been used, here K is the rate of reaction. For $k(T)$ it is common to use either Arrhenius kinetics or Heaviside kinetics:

$$k(T) = \begin{cases} 1 & \text{if } T \geq T_i \\ 0 & \text{otherwise.} \end{cases} \tag{52}$$

Henceforth Heaviside kinetics is used. It is also assumed that the specific heats at constant pressure of the two mixtures satisfies

$$C_{pa} = C_{pb} = C_p \tag{53}$$

where C_p is constant. This assumption yields

$$h = h_a Y + h_b Z = (h_a^0 - h_b^0)Y + h_b^0 + C_p T. \tag{54}$$

Here h_a^0 and h_b^0 are the heat of formation of mixture a and b respectively, let $Q = h_a^0 - h_b^0$. Furthermore it is assumed that the molecular masses of the two mixtures are the same (i.e. $W_a = W_b$). Hence, the equation of state for a perfect gas becomes

$$p = R_u T \rho(\frac{Y}{W_a} + \frac{Z}{W_b}) = RT\rho. \tag{55}$$

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Where R_u is the universal gas constant and $R = \frac{R_u}{W_a} = \frac{R_u}{W_b}$.

The following nondimensional variables are introduces

$$\hat{\rho} = \frac{\rho}{\rho_1}, \ \hat{x} = x\frac{\sqrt{Q}\rho_1}{\mu}, \ \hat{t} = t\frac{Q\rho_1}{\mu}, \ \hat{u} = \frac{u}{\sqrt{Q}} \qquad (56)$$

and

$$\hat{T} = T\frac{C_p}{Q}, \ \hat{h} = \frac{h}{Q}, \ \hat{p} = \frac{p}{Q\rho_1}, \ \hat{k}(\hat{T}) = k(T). \qquad (57)$$

Here ρ_1 is the density at the unburnt side. Eqs.(47,48) become

$$(\hat{\rho})_{\hat{t}} + (\hat{\rho}\hat{u})_{\hat{x}} = 0 \qquad (58)$$

and

$$(\hat{\rho}\hat{u})_{\hat{t}} + (\hat{\rho}\hat{u}^2 + \hat{p})_{\hat{x}} - \hat{u}_{\hat{x}\hat{x}} = 0 \qquad (59)$$

respectively. The nondimensionalizing of the energy equation yields

$$\hat{\rho}(\hat{h} + \frac{\hat{u}^2}{2})_{\hat{t}} + \hat{\rho}\hat{u}(\hat{h} + \frac{\hat{u}^2}{2})_{\hat{x}} - \hat{p}_{\hat{t}} = (\hat{u}\hat{u}_{\hat{x}})_{\hat{x}} \qquad (60)$$

The equation of state becomes

$$\hat{p} = \frac{\gamma - 1}{\gamma}\hat{\rho}\hat{T} \qquad (61)$$

where

$$\gamma = \frac{C_p}{C_v} \text{ and } C_p - C_v = R. \qquad (62)$$

The enthalpy gets the form

$$\hat{h} = Y + \hat{h}_b^0 + \hat{T}. \qquad (63)$$

Finally, Eq.(50) becomes

$$(\hat{\rho}Y)_{\hat{t}} + (\hat{\rho}\hat{u}Y)_{\hat{x}} = -\frac{\mu K}{Q\rho_1}\hat{k}(\hat{T})\hat{\rho}Y. \qquad (64)$$

If the hats over the variables are neglected the system becomes

$$\rho_t + (\rho u)_x = 0, \qquad (65)$$
$$(\rho u)_t + (\rho u^2 + p)_x - u_{xx} = 0, \qquad (66)$$
$$\rho(h + \frac{u^2}{2})_t + \rho u(h + \frac{u^2}{2})_x - p_t = (u u_x)_x, \qquad (67)$$
$$(\rho Y)_t + (\rho u Y)_x = -Kr k(T)\rho Y \qquad (68)$$

and

$$h = Y + h_b^0 + T \text{ and } p = \frac{\gamma - 1}{\gamma}\rho T. \qquad (69)$$

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Here the dimensionless number Kr, the *Kreiss number*

$$Kr = \frac{\mu K}{Q \rho_1} \tag{70}$$

has been introduced. Henceforth only the nondimensional variables will be considered. In Eqs.(65-68) all variables are functions of x and t, the one space coordinate and time. Introducing a moving coordinate system, $z = x + st$, s constant, yields

$$\rho_t + s\rho_z + (\rho u)_z = 0, \tag{71}$$

$$(\rho u)_t + s(\rho u)_z + (\rho u^2 + p)_z - u_{zz} = 0, \tag{72}$$

$$\rho(h + \frac{u^2}{2})_t + \rho s(h + \frac{u^2}{2})_z + \rho u(h + \frac{u^2}{2})_z - p_t - sp_z = (uu_z)_z, \tag{73}$$

$$(\rho Y)_t + s(\rho Y)_z + (\rho u Y)_z = -Krk(T)\rho Y. \tag{74}$$

After it has been assumed that the variables are independent of time in this moving coordinate system the equations can (after some algebra) be rewritten in the form

$$(\rho(s + u))_z = 0, \tag{75}$$

$$(\rho(s + u)^2 + p)_z - u_{zz} = 0, \tag{76}$$

$$(\rho(s + u)(h + \frac{(s + u)^2}{2}))_z = ((s + u)u_z)_z, \tag{77}$$

$$(\rho(s + u)Y)_z = -Krk(T)\rho Y. \tag{78}$$

Eq.(75-77) can be integrated,

$$\rho(s + u) = c_1, \tag{79}$$

$$\rho(s + u)^2 + p - u' = c_2, \tag{80}$$

$$\rho(s + u)(h + \frac{(s + u)^2}{2}) - (s + u)u' = c_3, \tag{81}$$

where $' = \partial/\partial z$. In the same way as in [6] the new variable $v = 1/\rho$ (the specific volume) is introduced into Eq.(79), yielding

$$v = \frac{s + u}{c_1} \tag{82}$$

and

$$u' = c_1 v'. \tag{83}$$

Use of this give

$$v' = \frac{1}{c_1}[\frac{\gamma - 1}{\gamma}\frac{T}{v} + c_1^2(v - a)], \tag{84}$$

$$0 = c_1[Y + h_i^0 + T - \frac{1}{2}c_1^2(v - a)^2 - c - \frac{\gamma - 1}{\gamma}T], \tag{85}$$

$$c_1 Y' = -Krk(T)\frac{1}{v}Y, \tag{86}$$

where

$$a = c_2/c_1^2 \text{ and } c = \frac{c_3}{c_1} - \frac{1}{2}\frac{c_2^2}{c_1^2} \qquad (87)$$

and Eq.(69) has been used for the pressure and the enthalpy. The next step is to use the conditions at the low temperature side, before the detonation, to determine the constants of integration from Eq.(79)-(81). It will be assumed that $u = 0$, $T = T_1$ and $Y = Y_1$ (from Eq.(56) $v = 1$) there. This give

$$c_1 = s, \qquad (88)$$

$$c_2 = s^2 + \frac{\gamma - 1}{\gamma}T_1, \qquad (89)$$

$$c_3 = s(Y_1 + h_b^0 + T_1 + \frac{s^2}{2}). \qquad (90)$$

Hence

$$a = \frac{c_2}{c_1^2} = (1 + \frac{\gamma - 1}{\gamma}\frac{T_1}{s^2}) \qquad (91)$$

and

$$c = \frac{c_3}{c_1} - \frac{1}{2}\frac{c_2^2}{c_1^2} = Y_1 + h_b^0 + \frac{1}{\gamma}T_1 - \frac{1}{2}\frac{1}{s^2}(\frac{\gamma - 1}{\gamma}T_1)^2. \qquad (92)$$

Use of these constants give

$$T = \frac{1}{2}s^2\gamma v^2 - (\gamma s^2 + \gamma T_1 - T_1)v + \frac{1}{2}\gamma s^2 + \gamma T_1 + \gamma(Y_1 - Y) \qquad (93)$$

and

$$v' = \frac{1}{sv}[\frac{1}{2}s^2(\gamma + 1)v^2 - (\gamma s^2 + (\gamma - 1)T_1)v + (\gamma - 1)(\frac{1}{2}s^2 + T_1 + (Y_1 - Y))]. \qquad (94)$$

Or by introducing

$$p(v; s^2) = \frac{1}{\gamma - 1}[\frac{1}{2}s^2(\gamma + 1)v^2 - (\gamma s^2 + (\gamma - 1)T_1)v + (\gamma - 1)(\frac{1}{2}s^2 + T_1 + Y_1)], \qquad (95)$$

$$q(v; s^2) = \frac{1}{2}s^2v^2 - (s^2 + T_1 - \frac{T_1}{\gamma})v + \frac{1}{2}s^2 + T_1 + Y_1 - \frac{1}{\gamma}T_i \qquad (96)$$

the system of equations becomes finally

$$v' = \frac{1}{sv}(\gamma - 1)(p(v; s^2) - Y), \qquad (97)$$

$$Y' = -KrH(T - T_i)\frac{1}{sv}Y, \qquad (98)$$

and

$$T = \gamma(q(v; s^2) - Y) + T_i. \qquad (99)$$

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B Extension of Proofs for the Chapman-Jouget Detonation

The critical point $(v_c, 0)$ is not hyperbolic, and therefore the linearized analysis can not be used to derive the slope of the monotonic solution at that point, instead the following method is used. Eqs.(7,8) become

$$v' = \frac{1}{sv}(\gamma - 1)(\alpha(v - v_c)^2 - Y) \tag{100}$$

$$Y' = -Kr\frac{1}{sv}Y \tag{101}$$

on and below the curve $Y = q(v; s^2)$. Eq.(15) shows that

$$\alpha = \frac{1}{2}s^2\frac{\gamma + 1}{\gamma - 1}. \tag{102}$$

Now $x = v - v_c$ is introduced. Y is a monotonic function of z, hence x can be considered as a function of Y satisfying the equation

$$\frac{dx}{dY} = \frac{\gamma - 1}{Kr}\frac{Y - \alpha x^2}{Y}. \tag{103}$$

Since $Y \geq 0$ and $\alpha > 0$ the following must hold

$$Y - \alpha x^2 \leq Y \tag{104}$$

which implies

$$\frac{Y - \alpha x^2}{Y} \leq 1. \tag{105}$$

From lemma 4 it is known that the solution under consideration approaches the critical point from the interior of the parabola $Y = p(v; s^2)$, and hence $Y - \alpha x^2 \geq 0$. Eq.(103) then provides the following bound on the derivative

$$0 \leq \frac{dx}{dY} \leq \frac{\gamma - 1}{Kr}. \tag{106}$$

These inequalities, which are valid even at the critical point for the solution under consideration, gives the following bound

$$0 \leq x(Y) \leq \frac{\gamma - 1}{Kr}Y. \tag{107}$$

(Or more precisely, integration from δ to Y give

$$x(\delta) \leq x(Y) \leq x(\delta) - \frac{\gamma - 1}{Kr}\delta + \frac{\gamma - 1}{Kr}Y. \tag{108}$$

Since

$$0 \leq x(\delta) \leq \sqrt{\frac{\delta}{\alpha}} \tag{109}$$

and since δ is arbitrary the inequality in Eq.(107) is obtained.)

The right inequality can be used to get a better estimate for the slope, and as above one gets

$$\frac{Y - \alpha x^2}{Y} \geq 1 - \alpha(\frac{\gamma - 1}{Kr})^2 Y \tag{110}$$

which together with Eq.(106) leads to

$$\frac{\gamma - 1}{Kr}(1 - \alpha(\frac{\gamma - 1}{Kr})^2 Y) \leq \frac{dx}{dY} \leq \frac{\gamma - 1}{Kr} \tag{111}$$

from which it is realized that

$$\lim_{Y \to 0} \frac{dx}{dY} = \frac{\gamma - 1}{Kr}. \tag{112}$$

The inequality above also yields

$$x(Y) = \frac{\gamma - 1}{Kr} Y + O(Y^2). \tag{113}$$

Next it is shown that this monotonic solution is unique. Assume that there are two solutions for the same Kr_{cr}, let them be denoted by $\psi_1(Y)$ and $\psi_2(Y)$. Introduce $\psi = \psi_1 - \psi_2$, hence

$$\frac{d\psi}{dY} = \frac{\gamma - 1}{Kr_{cr}}(\frac{Y - \alpha \psi_1^2}{Y} - \frac{Y - \alpha \psi_2^2}{Y}) \tag{114}$$

or

$$\frac{d\psi}{dY} = -\frac{\gamma - 1}{Kr_{cr}} \alpha \frac{1}{Y}(\psi_1^2 - \psi_2^2) \tag{115}$$

or

$$\frac{d\psi}{dY} = -\beta \frac{\psi_1 + \psi_2}{Y} \psi \quad \text{where} \quad \beta = \alpha \frac{\gamma - 1}{Kr_{cr}}. \tag{116}$$

From Eq.(113) it follows that for small values of Y this can be written

$$\frac{d\psi}{dY} = -2\beta \frac{\gamma - 1}{Kr_{cr}}(1 + O(Y))\psi, \tag{117}$$

which contradicts the fact that $\psi(Y) \to 0$ as $Y \to 0$.

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