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One-Dimensional Detonation Waves

by

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The Numerical Computation of
One-Dimensional Detonation Waves

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Abstract

In this paper we consider the numerical computation of one-dimensional detonation waves. Detonation waves are travelling wave solutions of the reactive Euler equations. An essential numerical difficulty in the numerical computation of detonation waves is the occurrence of completely wrong wave speeds, corresponding with non-physical solutions of the reactive Euler equations. The numerical propagation speed is strongly influenced by the choice of the ignition temperature. In this paper it is proved that non-physical solutions are always weak detonation waves. Furthermore, we present theoretical insights assessing why a correct ignition temperature will exclude non-physical weak detonation waves, just like the entropy condition excludes non-physical expansion shocks in the non-reacting case. This is illustrated by numerical computations quite well.

A.M.S. Classifications: 35L60, 35L65, 65M06
Keywords: Conservation laws, reactive Euler equations, detonation waves, ZND-model, numerical wave speed.
1 Introduction

In the flow of a reacting gas mixture, chemical reactions between the constituent gases need to be modelled together with the fluid dynamics. Problems of this form arise, for example, in combustion [8, 17, 18]. The basic equations of combustion theory are the conservation equations for reacting gas flow together with chemical kinetics. These equations represent the conservation of mass, momentum and energy of the total mixture and the conservation of mass for the various species.

A considerable simplification of these equations is possible if we restrict ourselves to one-dimensional detonations. For detonation waves, energy release occurs so quickly that molecular diffusion, thermal conductivity and viscosity are usually unimportant transport mechanisms, and therefore they are ignored. If effects of walls, heat sources and external forces are also ignored, we essentially obtain the Euler equations of gas dynamics, completed with the continuity equations for the various species. These latter equations include source terms, which describe the chemical reactions. Generally, the chemical reactions are described by the ignition model, the law of mass action and Arrhenius's law [17, 18]. The total system of equations is often referred to as the reactive Euler equations.

When attempting to solve the reactive Euler equations numerically, we encounter problems that are absent in non-reacting flows. Apart from an increase in the number of equations, the main difficulty is the fact that, in general, the time-scales of the chemical reactions are very small compared to the time-scale of the fluid dynamics. For fast reactions it is possible to obtain stable numerical solutions that look reasonable and yet are completely wrong, because the discontinuities have the wrong locations. Thus, the numerical reaction waves are propagating at non-physical wave speeds [6]. A detailed analysis of the numerical wave speed for (scalar) model problems is given in several papers (cf. e.g. [2, 9, 12, 13]). For several scalar model problems it has been shown that the ignition value for the chemical reaction plays a crucial role in obtaining correct numerical wave speeds [2].

In this paper we consider detonation waves described by the ZND-model [8, 17]. The ZND-model assumes that the detonation wave consists of an ordinary non-reacting shock wave followed by a reaction zone. Hence, due to a precursor shock wave the temperature jumps to a value larger than the ignition temperature and a reaction is started.

We want to study the influence of the ignition temperature on the numerical wave speed. For the ZND-solution of detonation waves, it is realistic to choose the ignition temperature equal to the value of the temperature just behind the ordinary shock wave, since the ZND-theory assumes that no reaction takes place in front of this non-reacting shock wave. We shall refer to this ignition temperature as the correct ignition temperature. However, several authors have chosen the ignition temperature much smaller [6, 9, 12]. In this way the problem is made highly sensitive to numerical diffusion. The numerical diffusion in front of the non-reacting shock wave starts an artificial reaction and therefore causes a considerable increase of the numerical wave speed. Hence, the choice of the ignition temperature seems to play an important role.

It is well known that for the non-reacting Euler equations it is also possible to obtain shock waves propagating at non-physical wave speeds. These non-physical solutions are expansion shocks and are, in general, excluded by adding an extra condition to the numerical method, namely the entropy condition [1, 10, 16].

For the reactive Euler equations we have essentially the same problem. In this paper we show that these non-physical solutions are always weak detonation waves. It follows from Jouguet's rule [7] that for weak detonation waves the characteristics behind the shock wave are coming out of the shock wave, which is similar to expansion shocks for the ordinary
Euler equations. We present theoretical insights assessing why a correct ignition temperature will exclude non-physical weak detonation waves, just like the entropy condition excludes non-physical expansion shocks in the non-reacting case. This is illustrated by numerical computations quite well.

This paper is organized as follows. In the next section one-dimensional hyperbolic conservation laws with source terms are introduced. Furthermore, weak solutions of these equations are introduced. In Section 3 the reactive Euler equations are presented. The reactive Rankine-Hugoniot equations are introduced and the ZND-model is described. The well-known first order splitting method is presented in Section 4. We extend Roe's method to two-component gas flow. In the following section we prove two theorems. Firstly, it is shown that the numerical travelling wave solution has to satisfy the reactive Rankine-Hugoniot equations. Secondly, we prove that non-physical solutions are always weak detonation waves. In Section 6 we present some numerical results that illustrate the preceding analysis. Furthermore, using these results we explain the good results for correct ignition temperatures.

2 Hyperbolic Conservation Laws with Source Terms

In the following we consider one-dimensional conservation laws with source terms. It is assumed that the source terms are only dependent on the solution u. The general form of such conservation laws is

$$\frac{d}{dt} \int_{x_L}^{x_R} u(x,t) dx = f(u(x_L,t)) - f(u(x_R,t)) + \int_{x_L}^{x_R} q(u(x,t)) dx.$$  \hspace{1cm} (2.1)

Conservation laws of this form occur, among others, in the theory of reacting gas flow [7, 8, 17, 18]. Assume that the solution u : $\mathbb{R} \times [0, \infty) \rightarrow \mathbb{R}^m$ and the flux function f : $\mathbb{R}^m \rightarrow \mathbb{R}^m$ are continuously differentiable and let the source term q : $\mathbb{R}^m \rightarrow \mathbb{R}^m$ be continuous. Then, since (2.1) should hold for arbitrary $x_L$ and $x_R$, it is clear that u satisfies

$$\frac{\partial}{\partial t} u(x,t) + \frac{\partial}{\partial x} f(u(x,t)) = q(u(x,t)).$$  \hspace{1cm} (2.2a)

This is the differential form of the conservation law. In order to obtain an initial value problem we add initial data to (2.2a), i.e.

$$u(x, 0) = u^0(x), \ \forall x \in \mathbb{R}.$$  \hspace{1cm} (2.2b)

The assumption of the solution of (2.1) to be continuously differentiable is too strong, since in practice discontinuous solutions u of (2.1) also occur [8, 17]. This is the reason why weak solutions of the initial value problem (2.2) are interesting. These weak solutions are obtained from multiplying (2.2a) with an arbitrary test function $\varphi \in C^0_0(\mathbb{R} \times [0, \infty))$ (i.e. $\varphi$ vanishes for $|x| + t$ large) and, subsequently, partially integrating this equation in space and time. This leads to the following definition.

**Definition 2.1** A bounded measurable function u is called a weak solution of the conservation law (2.2a) with bounded initial data (2.2b) if

$$\int_0^\infty \int_{-\infty}^{\infty} \left\{ u(x,t) \frac{\partial}{\partial t} \varphi(x,t) + f(u(x,t)) \frac{\partial}{\partial x} \varphi(x,t) \right\} dx dt =$$

$$-\int_{-\infty}^{\infty} u^0(x) \varphi(x,0) dx - \int_0^\infty \int_{-\infty}^{\infty} q(u(x,t)) \varphi(x,t) dx dt$$

for all functions $\varphi \in C^0_0(\mathbb{R} \times [0, \infty)).$
From now on by a solution of (2.2) a weak solution of (2.2) in the sense of Definition 2.1 is meant. It can be shown that a solution of (2.1) is always a weak solution of (2.2).

A difficulty is that the weak solutions of (2.2) turn out to be non-unique for a given set of initial data, and it remains to characterise the "physically relevant" weak solution. For homogeneous conservation laws the usual criterion is to impose an extra condition upon the solution, the so-called *entropy condition*, such that a physically relevant solution is obtained [10]. However, to our knowledge for non-homogeneous conservation laws this is an open problem yet.

Next hyperbolic conservation laws with source terms are introduced. We start with introducing the quasi-linear form of the conservation law as

$$\frac{\partial}{\partial t} u(x, t) + A(u(x, t)) \frac{\partial}{\partial x} u(x, t) = q(u(x, t)),$$  

(2.4)

where $A(u)$ is the Jacobian matrix of $f(u)$, defined by

$$A(u) := \frac{\partial}{\partial u} f(u).$$  

(2.5)

There are cases in which the Jacobian matrix $A(u)$ is not defined for all $u \in \mathbb{R}^m$ and we have to restrict ourselves to a certain domain $\Omega \subset \mathbb{R}^m$. A hyperbolic conservation law with source term on $\Omega$ is defined as follows [1, 10].

**Definition 2.2** Let a domain $\Omega \subset \mathbb{R}^m$ be given, such that $A(u)$ is well defined by (2.5) for all $u \in \Omega$. The system (2.2a) is called a hyperbolic conservation law with source term on $\Omega$ if there exists a real diagonal matrix $\Lambda(u)$ and a non-singular real matrix $R(u)$ such that

$$A(u)R(u) = R(u)\Lambda(u). \quad \forall u \in \Omega.$$  

(2.6)

Here $\Lambda(u) = \text{diag}(\lambda_1(u), \lambda_2(u), \ldots, \lambda_m(u))$ is the diagonal matrix of the eigenvalues of $A(u)$ and $R(u) = (r^{(1)}(u), r^{(2)}(u), \ldots, r^{(m)}(u))$ is the matrix of the corresponding right eigenvectors of $A(u)$. We assume that the eigenvalues are labeled in nondecreasing order, i.e. $\lambda_1(u) \leq \lambda_2(u) \leq \ldots \leq \lambda_m(u)$.

A very important example of a system of hyperbolic conservation laws with source terms are the reactive Euler equations, which are described in the next section.

We conclude this section by considering discontinuous solutions of (2.1) in more detail. Let $u$ have a discontinuity along a smooth curve $\Gamma$, i.e. $u$ has well defined limits on both sides of $\Gamma$. Let $\Gamma$ be given by $x = x(t)$, then the values $u_L = u(x(t) - 0, t)$ and $u_R = u(x(t) + 0, t)$ are well defined. Suppose that the differential equation (2.2a) holds on both sides of $\Gamma$ and suppose that $x_L < x(t) < x_R$ for some fixed $t \geq 0$. Let $s = x'(t)$ be the speed of the discontinuity, then

$$\frac{d}{dt} \int_{x_L}^{x_R} u(x, t)dx = \frac{d}{dt} \left\{ \int_{x_L}^{x(t)} u(x, t)dx + \int_{x(t)}^{x_R} u(x, t)dx \right\}$$

$$= \int_{x_L}^{x(t)} \frac{\partial}{\partial t} u(x, t)dx + \int_{x(t)}^{x_R} \frac{\partial}{\partial t} u(x, t)dx + (u_L - u_R)s$$

$$= f(u(x_L, t)) - f(u_L) + f(u_R) - f(u(x_R, t)) + (u_L - u_R)s$$

$$+ \int_{x_L}^{x_R} q(u(x, t))dx.$$  

3
Thus, (2.1) shows that
\[ s(u_L - u_R) = f(u_L) - f(u_R) \] (2.7)
must hold at each point on \( \Gamma \). Relation (2.7) is called the jump condition. In non-reactive gas dynamics the system of equations (2.7) is known as the Rankine-Hugoniot equations.

3 The Reactive Euler Equations

3.1 Preliminaries

In this section we will describe a very important example of a system of hyperbolic conservation laws with source terms, namely the reactive Euler equations. For a more complete description, see e.g. [8, 17].

Consider a tube filled with a gas mixture, which is uniformly distributed across the tube, so there is variation in only one direction and we can restrict ourselves to one space dimension. For the sake of simplicity we assume that the gas is a binary mixture in which only one chemical reaction takes place. Thus, consider the one-step reaction \( R \rightarrow P \), where \( R \) is the reactant and \( P \) is the product. Further assume that a detonation wave is propagating in the positive \( x \)-direction. Ahead of the detonation wave there is a reactant. In the detonation wave the gas is burnt and the reactant is entirely converted into the product. All quantities ahead of the detonation wave will be identified by the subscript \( u \) (the unburnt gas), while the quantities behind the wave are denoted by the subscript \( b \) (the burnt gas).

For detonation waves the general combustion equations simplify to the reactive Euler equations. These equations represent the conservation of mass, momentum and energy of the total mixture and the conservation of mass for the reactant. The latter equation includes a source term which describes the chemical reaction that takes place.

With mass density \( \rho \), mass-weighted average velocity \( u \), pressure \( p \), specific total energy \( E \), specific stagnation enthalpy \( H \), mass fraction of reactant \( Y \) and reaction rate \( w \), the one-dimensional reactive Euler equations are

\[
\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) = 0, \tag{3.1a}
\]
\[
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) = 0, \tag{3.1b}
\]
\[
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x}(\rho uH) = 0, \tag{3.1c}
\]
\[
\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial x}(\rho uY) = w, \tag{3.1d}
\]
where the stagnation enthalpy \( H \) is defined by

\[ H := E + \frac{p}{\rho}. \tag{3.2} \]

All variables have been made dimensionless by normalizing them with respect to some reference state. To complete the system (3.1), the pressure \( p \) and the reaction rate \( w \) have to be related to the independent variables \( \rho, u, E \) and \( Y \). If we assume that both gases behave like an ideal gas with the same specific heat ratio \( \gamma \), then the thermodynamic identity is given by

\[ p = (\gamma - 1)\rho(E - \frac{1}{2}u^2 - QY), \tag{3.3} \]
where \( Q > 0 \) is the heat release of the chemical reaction. Next we specify how the reaction rate \( w \) depends on the other variables. We assume that the one-step reaction is described by the ignition model, the law of mass action and Arrhenius' law [17, 18]

\[
 w := \begin{cases} 
 -D_o \rho Y \exp\left(\frac{E_o}{T_{eN}} - \frac{1}{T}\right) & \text{if } T \geq T_{ign}, \\
 0 & \text{if } T < T_{ign}, 
\end{cases}
\]

(3.4)

where \( E_o \) is the activation energy, \( T_{eN} \) is the von Neumann temperature, which is discussed in Section 3.3, \( T_{ign} \) is the ignition temperature and \( Da \) is referred to as the Damköhler number.

The ignition temperature satisfies \( T_n < T_{ign} \leq T_{eN} \). The Damköhler number is defined by the ratio of the convection length scale and the reaction length scale [17]. Obviously, if \( Da \) is small the reaction occurs slowly relative to the specified time scale and if \( Da \) is large, the reaction zone is thin and the reaction occurs quickly relative to the specified time scale. Equation (3.4) defines \( w \) as a function of \( \rho, u, E \) and \( Y \) through the thermodynamic identity (3.3) and the equation of state

\[
p = \rho T.
\]

(3.5)

The system of equations (3.1), (3.2), (3.3), (3.4) and (3.5) consists of eight equations for the variables \( \rho, u, E, Y, p, H, T, \) and \( w \).

If the vector of conservative variables \( u \), the flux vector \( f(u) \) and the source vector \( q(u) \) are defined by, respectively,

\[
 u := (\rho, \rho u, \rho E, \rho Y)^T,
\]

\[
f(u) := (\rho u, \rho u^2 + p, \rho uH, \rho uY)^T,
\]

\[
 q(u) := (0, 0, 0, w)^T.
\]

(3.6)

then the reactive Euler equations can be written in the general form (2.2a).

Let the Jacobian matrix \( A(u) \) be defined as in (2.5). For the reactive Euler equations the eigenvalues \( \lambda_i \) and right eigenvectors \( r^{(i)}(u) \), \( i = 1, \ldots, 4 \), of \( A(u) \) are given by

\[
 \lambda_1(u) = u - c, \quad \lambda_2(u) = u, \quad \lambda_3(u) = u, \quad \lambda_4(u) = u + c,
\]

(3.7)

and

\[
 r^{(1)}(u) = (1, u - c, H - uc, Y)^T,
\]

\[
 r^{(2)}(u) = (1, u, \frac{1}{2} u^2, 0)^T,
\]

\[
 r^{(3)}(u) = (0, 0, Q, 1)^T,
\]

\[
 r^{(4)}(u) = (1, u + c, H + uc, Y)^T.
\]

(3.8)

In (3.7) and (3.8), \( c \) is the frozen speed of sound, which for an ideal gas is given by

\[
c = \sqrt{\frac{T_p}{\rho}}.
\]

(3.9)

Obviously, the reactive Euler equations are a hyperbolic system of conservation laws with source terms.
### 3.2 Reacting Shock Waves

Often the Damköhler number $Da$ is very large, i.e. the reaction length is very small relative to the convection length. We start with considering the limit $Da \to \infty$, in which case the reactant is converted into the product instantaneously. For this limit the combustion waves are often called reacting shock waves.

The reactive Rankine-Hugoniot equations relate the state of the unreacted gas ahead of the reacting shock wave with the state of the completely reacted gas, behind the reacting shock wave for a given wave speed $s$. These equations are derived in a similar way as the ordinary Rankine-Hugoniot equations for non-reacting shock waves. It is clear that $s > u_u$ and $s > u_b$, since otherwise the wave will never pass the unburnt gas.

Since the reacting shock wave is propagating with a constant speed $s$ through the tube, it is natural to introduce a coordinate system which is stationary with respect to the wave. Therefore, the variable $\xi$ is introduced as

$$\xi(x, t) := x - sl. \quad (3.10)$$

Using (3.10) we write $g(x, t) = g(x - sl) = g(\xi)$ for all variables $g$. Subsequently, (3.1) can be rewritten as a system of ordinary differential equations, i.e.

$$-s \frac{d}{d\xi} u(\xi) + \frac{d}{d\xi} f(u(\xi)) = q(u(\xi)), \quad (3.11)$$

where $u$, $f(u)$ and $q(u)$ are given by (3.6). After integrating (3.11) from $\xi = -\infty$ to $\xi = +\infty$, we deduce

$$s(u_b - u_u) = f(u_b) - f(u_u) + \int_{-\infty}^{+\infty} q(u(\xi))d\xi. \quad (3.12)$$

The first three equations of (3.12), for which the integral vanishes, are called the reactive Rankine-Hugoniot equations. Further note that if no reaction takes place (i.e. $q = 0$), then (3.12) reduces to the ordinary Rankine-Hugoniot equations (2.7).

For details concerning these equations the reader is referred to e.g. [7, 8, 17, 18]. In this paper we just summarize some results obtained from the reactive Rankine-Hugoniot equations.

Firstly, we can distinguish two types of reacting shock waves, namely detonation waves and deflagration waves. If a detonation wave passes the unburnt gas, the pressure and the density jump to higher values (i.e. $p_b > p_u$ and $\rho_b > \rho_u$). On the other hand if a deflagration wave passes the unburnt gas the pressure and the density jump to lower values (i.e. $p_b < p_u$ and $\rho_b < \rho_u$). Secondly, the gas flow is supersonic relative to the reaction front ahead of a detonation wave (i.e. $s - u_u > c_u$) and subsonic relative to the reaction front ahead of a deflagration wave (i.e. $s - u_u < c_u$). In this paper we restrict ourselves to detonation waves.

Subsequently, detonation waves can be distinguished in three different types namely, strong, Chapman-Jouguet and weak detonation waves. We present, without proof, some characteristic properties by which we can distinguish the various detonation waves. These properties are referred to as Jouguet’s rule [7].

**Jouguet’s Rule:**

The gas flow relative to the reaction front is

- supersonic ahead of a detonation front (i.e. $s - u_u > c_u$),
- subsonic behind a strong detonation front (i.e. $0 < s - u_b < c_b$),
sonic behind a Chapman-Jouguet detonation front (i.e. $s - u_b = c_b$),

supersonic behind a weak detonation front (i.e. $s - u_b > c_b$).

The Chapman-Jouguet (CJ) detonation wave is of particular importance since this wave travels with the minimal speed of all the possible detonation waves [7, 18]. Finally, it can be shown that weak detonations are only possible under extreme and rare circumstances [7, 18].

3.3 The ZND-Model for Detonation Waves

The previous considerations give no insight into the internal structure of detonation waves, since $Da$ was assumed to be infinitely large. For finite Damkohler numbers we expect some region of finite width across which the reaction takes place. Independently from each other, Zeldovich, von Neumann and Döring developed a model which explains the internal structure of detonation waves, the so-called ZND-model [7, 8, 17]. The ZND-model assumes the following.

A detonation wave travelling with constant speed $s$ has the internal structure of an ordinary (non-reacting) precursor fluid dynamical shock wave followed by a deflagration wave.

The reaction rate is zero ahead of the shock and finite behind.

Hence, due to a non-reacting shock wave the temperature of the unburnt gas $T_u$ jumps to a value larger than $T_{\text{ign}}$ and a reaction is started. The values immediately behind the non-reacting shock wave are called the von Neumann values and would be the final values if no chemical reaction takes place. For instance, the temperature behind the ordinary shock wave is called the von Neumann temperature $T_{\text{vN}}$, which is used in the definition of the reaction rate $w$ (3.4). As the reaction proceeds (through the deflagration wave) $Y$ decreases from 1 to 0 and the pressure and density decrease to their final values $p_b$ and $\rho_b$, respectively. An example of a ZND-profile is given in Figure 1. In this figure the ordinary shock wave is located at $\xi = 0$.

Using the reactive Rankine-Hugoniot equations and the ZND-model we can derive algebraic expressions which express all variables in terms of $Y$ and, subsequently, also the reaction rate $w$ [8, 17]. Suppose that at time $t = 0$ the precursor shock is located at $x = 0$. Hence, at time $t$ the variable $\xi = x - st$ measures the distance between the point $x$ and the precursor shock. Therefore, $y(\xi) = y_0$ for all $\xi > 0$ and all variables $y$. Since the detonation wave is propagating with a constant speed $s > 0$, the mass fraction of the reactant $Y$ is given by the following ordinary differential equation [3, 8, 17]:

$$\frac{d}{d\xi} Y(\xi) = -\frac{w[Y(\xi)]}{m}, \quad \forall \xi < 0, \quad (3.13a)$$

$$Y(0) = 1, \quad (3.13b)$$

where $\xi = 0$ corresponds to the position of the precursor shock and $m = \rho_u(s - u_u) > 0$ is the mass flux. In general, (3.13) cannot be solved exactly and the solution must be computed numerically. The ZND-model can only describe strong or CJ detonations. Therefore, we restrict ourselves to strong or CJ detonations [7, 17].

As mentioned before, the minimum speed for a detonation is the speed $s_{\text{CJ}}$ of a CJ detonation [7, 8, 17]. It will be useful to define a quantity which measures the overdrive of a strong detonation. Therefore, let the degree of overdrive $f$ be defined by [4]

$$f := \left(\frac{s}{s_{\text{CJ}}}\right)^2. \quad (3.14)$$
from which it directly follows that \( f \geq 1 \). Finally, it is convenient to introduce the half-reaction length \( L_{1/2} \). The half reaction length is the distance for half completion of the reaction starting from the front of the detonation wave [8]. Often \( L_{1/2} \) is given and (3.4) is used to compute the corresponding Damköhler number \( Da \) [4, 8]. It is easy to see that (3.13) implies that \( L_{1/2} \) is given by

\[
L_{1/2} = -m \int_{1/2}^{1} \frac{1}{w(Y)} \, dY.
\]

(3.15)

In general, the half reaction length has to be computed by some numerical integration method, since it is not possible to solve the above integral exactly.

Ultimately, it is convenient to introduce the half-reaction length \( L_{1/2} \). The half reaction length is the distance for half completion of the reaction starting from the front of the detonation wave [8]. Often \( L_{1/2} \) is given and (3.4) is used to compute the corresponding Damköhler number \( Da \) [4, 8]. It is easy to see that (3.13) implies that \( L_{1/2} \) is given by

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\]

(3.15)

In general, the half reaction length has to be computed by some numerical integration method, since it is not possible to solve the above integral exactly.

Example 3.1 As an example of the preceding theory we describe the ZND-solution of the CJ detonation discussed in [3]. All quantities are non-dimensionalised with respect to the unburnt gas. Hence, the dimensionless preshock state is given by

\[
p_u = 1, \quad \rho_u = 1, \quad u_u = 0.
\]

Furthermore, we have the following parameter values:

\[
E_a = 14, \quad Q = 14, \quad f = 1, \quad \gamma = 1.4.
\]

Finally, \( L_{1/2} = 1 \) and the corresponding Damköhler number \( Da = 0.6488 \). We choose a relatively small \( Da \), since otherwise the reaction is very fast and the plot of the ZND-profile is

![Figure 1: ZND-solution of (3.1), with \( E_a = 14, Q = 14, f = 1, \gamma = 1.4 \) and \( Da = 0.6488 \).](image-url)
not very clarifying. The final state for the CJ detonation is given by

\[ p_b = p_{CJ} = 12.756, \quad p_b = \rho_{CJ} = 1.6583, \]
\[ u_b = u_{CJ} = 2.1602, \]

where the CJ detonation is propagating with a speed \( s = s_{CJ} = 5.4419 \). In Figure 1 the steady ZND-solution is drawn. The pressure reaches its maximum value right behind the precursor shock. As mentioned before the pressure in this point is called the von Neumann pressure, which in this particular case satisfies \( p_{vN} = p(0) = 24.512 \). For this particular example the von Neumann temperature is given by \( T_{vN} = 5.0509 \). Finally, \( c_b = 3.2817 \) and, subsequently, \( s - u_b = c_b \), as predicted by Jouguet’s rule.

4 A First Order Splitting Method

4.1 Introduction

A variety of numerical methods can be developed for conservation laws with source terms. A very natural way to solve (2.2) is a splitting method. In the splitting method the numerical solution at each time level is derived by a two step procedure. In the first step we approximate the solution of the homogeneous conservation law without the source term, i.e.

\[ \frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} f(u(x, t)) = 0. \tag{4.1} \]

In the second step we assume no convection (only reaction) and the following equation is solved numerically

\[ \frac{\partial}{\partial t} u(x, t) = q(u(x, t)). \tag{4.2} \]

There are several reasons for studying first order splitting methods. Firstly, the splitting method is interesting since good numerical methods exist for both subproblems (4.1) and (4.2). Furthermore, this method lends itself for thorough analysis. Finally, second order accuracy can be achieved using the Strang splitting [3, 15].

For a given time step \( \Delta t \), the discrete time levels \( t^n \) are defined by

\[ t^n := n\Delta t, \quad n = 0, 1, 2, \ldots. \]

For a given mesh width \( \Delta x \), the spatial mesh points \( x_i \) are defined by

\[ x_i := i\Delta x, \quad i = \ldots, -2, -1, 0, 1, 2, \ldots. \]

It will also be useful to define intermediate points

\[ x_{i+1/2} = (i + 1/2)\Delta x. \]

The average of \( u(\cdot, t^n) \) on the cell \([x_{i-1/2}, x_{i+1/2}]\) is defined by

\[ \bar{u}^n_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t^n) \, dx. \tag{4.3} \]

Note that the integral form of conservation laws describes the evolution in time of integrals such as (4.3). The finite difference methods we shall consider, produce approximations \( \bar{U}^n_i \in \mathbb{R}^m \).
of this average. In the following it is assumed that, for a given constant \( \tau > 0 \), the mesh width \( \Delta x \) and time step \( \Delta t \) satisfy
\[
\frac{\Delta t}{\Delta x} = \tau.
\]
We construct a piecewise constant function \( U_{\Delta t}(x, t) \) for all \( x \) and \( t \) from the discrete values \( U_i^n \) by
\[
U_{\Delta t}(x, t) = U_i^n, \quad \forall (x, t) \in [x_{i-1/2}, x_{i+1/2}) \times [t^n, t^{n+1}).
\] (4.4)

Next we describe in more detail the particular splitting method used in this paper. Suppose that the numerical solution at time level \( t^{n-1} \) (i.e. \( U_i^{n-1} \) for all \( i \)) is known and that we want to approximate the numerical solution at time level \( t^n \). In the first step we have to solve (4.1) numerically, which is done using a conservative \((2k+1)\)-point finite difference method with two time levels. Let us denote the result by \( C_i^n \), so
\[
C_i^n = U_i^{n-1} - \tau \{ F_{i+1/2}^{n-1} - F_{i-1/2}^{n-1} \},
\] (4.5)
where the numerical flux function \( F \) is a continuous function of the values of \( U \) at \( 2k \) points, i.e.
\[
F_{i+1/2}^{n-1} = F(U_{i+k}^{n-1}, \ldots, U_{i-k+1}^{n-1}).
\] (4.6)
For consistency we require that \( F \) satisfies
\[
F(v, \ldots, v) = f(v).
\] (4.7)
Further, it is assumed that (4.5) is an entropy stable method (cf. [1]). Hence, if (4.5) is applied to a homogeneous conservation law (i.e. \( q = 0 \)), then it will always approximate the unique physically relevant solution.

In the second step of the splitting method, we have to solve (4.2) numerically with initial data \( C_i^n \) given by (4.5). Hence, we have to approximate the solutions of the following initial value problems
\[
\frac{d}{dt} u(x_i, t) = q(u(x_i, t)), \quad t \in (t^{n-1}, t^n], \quad (4.8a)
\]
\[
u(x_i, t^{n-1}) = C_i^n. \quad (4.8b)
\]
The numerical solution of (4.8) is then defined as the numerical solution at time level \( t^n \) (i.e. \( U_i^n \) for all \( i \)). In realistic problems the time-scale of the chemical reaction is much smaller than the time-scale of the convection (i.e. the Damköhler number \( Da \) is large in (3.4)). Hence, for this kind of problems stability of a fully explicit method would imply a severe time step restriction and therefore (4.8) is solved by an implicit method. In this paper we use the backward Euler method, which results in
\[
U_i^n = C_i^n + \Delta t q(U_i^n). \quad (4.9)
\]

A straightforward combination of (4.5) and (4.9) shows that the total finite difference method reads
\[
U_i^n = U_i^{n-1} - \tau \{ F_{i+1/2}^{n-1} - F_{i-1/2}^{n-1} \} + \Delta tq(U_i^n). \quad (4.10)
\]
Many difficulties for a numerical method are caused by the fact that a discontinuous solution of (2.2) can occur. It is not surprising that the method might converge to the wrong solution, since in general a weak solution is not unique. More surprisingly a method may converge to a function that is not a weak solution at all. The following theorem shows that this problem is avoided by considering methods of type (4.10) only. Its proof is omitted since it is a straightforward extension of the well known theorem of Lax and Wendroff [11].
Theorem 4.1 Suppose that the finite difference method (4.10) has a continuous flux function \( F \) that satisfies (4.7) and a continuous source function \( q \). Let \( U^n_i \) be a solution of (4.10) with given initial values \( U^n_0 = u^n_0 \), as defined in (4.3). Define the piecewise constant function \( U_{\Delta t} \) as in (4.4). Suppose that there exists a sequence \( \Delta t_m \downarrow 0 \) as \( m \to \infty \) for which the limit

\[
\lim_{m \to \infty} U_{\Delta t_m}(x, t) = u(x, t)
\]

exists in the sense of bounded, \( L_1^{loc} \) convergence, i.e.

\[
\left\| U_{\Delta t_m} \right\|_{L_\infty(B \times [0, \infty))} \leq C,
\]

\( U_{\Delta t_m} \) converges towards \( u \) in \( L_1^{loc} \) as \( m \to \infty \).

Then the limit \( u \) is a weak solution of (2.2).

Note that the source term \( q \) should be continuous. However, (3.4) clearly illustrates that this requirement is not satisfied for the reactive Euler equations. Suppose that \( q \) is discontinuous in a point \( u_I \), then the proof can easily be generalized for this function \( q \) as long as \( \mu \{ (x, t) \in \Omega \mid u(x, t) = u_I \} = 0 \), where \( \Omega \subset B \times [0, \infty) \) is compact and \( \mu \) is the Lebesgue measure. However, for the sake of simplicity we have restricted ourselves to continuous source terms.

4.2 An extension of Roe’s method

In this paper the homogeneous conservation law is solved numerically using a first order Godunov-type method. In first order Godunov-type methods, the numerical solution is considered to be piecewise constant in each mesh cell \([x_{i-1/2}, x_{i+1/2})\) at a certain time level \( t^{n-1} = (n-1)\Delta t \). The evolution of the solution to the next time level \( t^n \) results from the wave interactions originating at the boundaries between adjacent cells. The cell interface at \( x_{i+1/2} \) separates two constant states \( U_i \) at the left and \( U_{i+1} \) at the right side, thus the resulting local interaction can be resolved exactly, since the initial conditions at time \( t^{n-1} \) correspond to the Riemann problem for a homogeneous conservation law. This problem has an exact solution consisting of constant states separated by shocks, contact discontinuities or simple waves \([1, 10]\). The new piecewise constant approximation at time \( t^n \) is then obtained by averaging the exact solution of the Riemann problem over each cell.

However, the computational costs to obtain this exact solution are generally high. Therefore, approximate Riemann solvers are considered in order to reduce the computational work. In this paper we have used the approximate Riemann solver developed by Roe \([14]\). However, all results remain valid for other approximate Riemann solvers.

Instead of solving the Riemann problem for the non-linear differential equation (4.1), Roe uses the exact solution of a locally linearized model in order to approximate the wave interactions originating at the boundaries of adjacent cells. Hence, each time step we solve the following Riemann problem exactly,

\[
\frac{\partial}{\partial t} \hat{U}_{i,n-1}(x, t) + \hat{A}(U_{i,n-1}, U_{i+1,n-1}) \frac{\partial}{\partial x} \hat{U}_{i,n-1}(x, t) = 0, \tag{4.11a}
\]

\[
\hat{U}_{i,n-1}(x, t^{n-1}) = \begin{cases} 
U_{i,n-1}, & x < x_{i+1/2}, \\
U_{i+1,n-1}, & x > x_{i+1/2}.
\end{cases} \tag{4.11b}
\]

where \( \hat{A}(U_{i,n-1}, U_{i+1,n-1}) \) is a constant \( m \times m \)-matrix. The matrix \( \hat{A} \) is required to satisfy the following properties:
(i) If \( U^n_{i+1}, U^n_{i+1} \rightarrow \bar{u} \), then \( \dot{A}(U^n_{i+1}, U^n_{i+1}) = A(\bar{u}) \);

(ii) \( \dot{A}(U^n_{i+1}, U^n_{i+1})(U^n_{i+1} - U^n_{i}) = f(U^n_{i+1}) - f(U^n_{i}) \);

(iii) \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \) is diagonalizable with real eigenvalues.

Condition (i) is necessary to recover the linearized algorithm from the non-linear version smoothly. Condition (ii) has two effects. Firstly it ensures the scheme to be conservative, and secondly, in the special case that \( U^n_{i+1} \) and \( U^n_{i+1} \) are connected by a single shock wave or contact discontinuity, the approximate Riemann solution agrees with the exact Riemann solution [14]. Finally, condition (iii) is clearly required for the problem to be hyperbolic and solvable. In the following it is assumed that there exists a matrix \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \), such that the conditions (i)-(iii) are satisfied.

Condition (iii) implies that there exists a real diagonal matrix \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \) and a non-singular real matrix \( \dot{R}(U^n_{i+1}, U^n_{i+1}) \) such that

\[
\dot{A}(U^n_{i+1}, U^n_{i+1}) \dot{R}(U^n_{i+1}, U^n_{i+1}) = \dot{R}(U^n_{i+1}, U^n_{i+1}) \dot{A}(U^n_{i+1}, U^n_{i+1}).
\]

Here \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \) is the matrix of the eigenvalues of \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \) and \( \dot{R}(U^n_{i+1}, U^n_{i+1}) \) is the matrix of the corresponding right eigenvectors of \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \). Hence,

\[
\dot{A}(U^n_{i+1}, U^n_{i+1}) = \text{diag}(\lambda_1(U^n_{i+1}, U^n_{i+1}), \lambda_2(U^n_{i+1}, U^n_{i+1}), \ldots, \lambda_m(U^n_{i+1}, U^n_{i+1})),
\]

\[
\dot{R}(U^n_{i+1}, U^n_{i+1}) = (\dot{r}^{(1)}(U^n_{i+1}, U^n_{i+1}), \dot{r}^{(2)}(U^n_{i+1}, U^n_{i+1}), \ldots, \dot{r}^{(m)}(U^n_{i+1}, U^n_{i+1})).
\]

For shortness of notation, \( \lambda_k(U^n_{i+1}, U^n_{i+1}) \) and \( \dot{r}^{(k)}(U^n_{i+1}, U^n_{i+1}) \) will simply be denoted by \( \lambda_k \) and \( \dot{r}^{(k)} \). For all \( k \) with \( 1 \leq k \leq m \), \( \lambda_k^+ \) and \( \lambda_k^- \) are defined by

\[
\lambda_k^+ = \max(\lambda_k, 0) \geq 0 \quad \text{and} \quad \lambda_k^- = \min(\lambda_k, 0) \leq 0. \tag{4.12}
\]

Since all eigenvectors are linearly independent the initial states \( U^n_{i+1} \) and \( U^n_{i+1} \) can be decomposed as

\[
U^n_{i+1} - U^n_{i+1} = \sum_{k=1}^{m} \hat{a}_k \dot{r}^{(k)}. \tag{4.13}
\]

where \( \hat{a}_k \in \mathbb{R} \) for all \( k \) with \( 1 \leq k \leq m \). Using this, it is straightforward that Roe's numerical flux is given by

\[
F^n_{i+\frac{1}{2}} = f(U^n_{i+1}) + \sum_{k=1}^{m} \lambda_k^- \hat{a}_k \dot{r}^{(k)}. \tag{4.14}
\]

It remains to compute a matrix \( \dot{A}(U^n_{i+1}, U^n_{i+1}) \) for the reactive Euler equations. It can be shown that for every pair \((U^n_{i+1}, U^n_{i+1})\) the matrix \( \dot{A} \) is given by

\[
\dot{A}(U^n_{i+1}, U^n_{i+1}) = \begin{pmatrix}
0 & 1 & 0 & 0 \\
\frac{1}{2} (\gamma - 3) \bar{u}^2 & (3 - \gamma) \bar{u} & \gamma - 1 & - (\gamma - 1) Q \\
\bar{u}(\frac{1}{2} (\gamma - 1) \bar{u}^2 - \bar{H}) & \bar{H} & (\gamma - 1) \bar{u}^2 & \gamma \bar{u} & - (\gamma - 1) Q \bar{u} \\
- \bar{u} \dot{Y} & \dot{Y} & 0 & \bar{u}
\end{pmatrix}, \tag{4.15}
\]
where the quantities \( \hat{u} \), \( \hat{H} \) and \( \hat{Y} \) are defined as

\[
\hat{u} = \frac{(u \sqrt{\rho})_{i+1}^{n-1} + (u \sqrt{\rho})_i^{n-1}}{\sqrt{\rho_{i+1}^{n-1} + \rho_i^{n-1}}}, \quad \hat{H} = \frac{(H \sqrt{\rho})_{i+1}^{n-1} + (H \sqrt{\rho})_i^{n-1}}{\sqrt{\rho_{i+1}^{n-1} + \rho_i^{n-1}}},
\]

\[
\hat{Y} = \frac{(Y \sqrt{\rho})_{i+1}^{n-1} + (Y \sqrt{\rho})_i^{n-1}}{\sqrt{\rho_{i+1}^{n-1} + \rho_i^{n-1}}}. \tag{4.16}
\]

In order to derive the eigenvectors and the eigenvalues of the matrix \( \hat{A}(U_i^{n-1}, U_{i+1}^{n-1}) \) the following quantity is useful. Define

\[
\hat{\epsilon}^2 = (\gamma - 1)(\hat{H} - \frac{\hat{u}^2}{2} - Q \hat{Y}). \tag{4.17}
\]

Now the computation of the eigenvalues and the eigenvectors is straightforward. They are given by

\[
\hat{\lambda}_1 = \hat{u} - \hat{\epsilon}, \quad \hat{\lambda}_2 = \hat{u}, \quad \hat{\lambda}_3 = \hat{u} + \hat{\epsilon}, \quad \hat{\lambda}_4 = \hat{u} + \hat{\epsilon}, \quad \hat{\lambda}_4 = \hat{u} - \hat{\epsilon},
\]

and

\[
\hat{\epsilon}^{(1)} = (1, \hat{u}, \hat{H}, \hat{\epsilon}), \quad \hat{\epsilon}^{(2)} = (1, \hat{u}, \frac{1}{2} \hat{u}^2, 0), \quad \hat{\epsilon}^{(3)} = (0, 0, Q, 1), \quad \hat{\epsilon}^{(4)} = (0, \hat{u} + \hat{\epsilon}, \hat{H} + \hat{u} \hat{\epsilon}, \hat{Y}). \tag{4.19}
\]

Hence, for every pair \((U_i^{n-1}, U_{i+1}^{n-1})\) Roe’s numerical flux \( F_{i+1/2}^{n-1} \) at the cell interface \( x_{i+1/2} \) is derived by a four-step procedure. The first step is the computation of the quantities defined in (4.16) and (4.17). In the second step the eigenvalues (4.18) and eigenvectors (4.19) are computed. Finally, in the third step, (4.13) is used to compute \( \hat{\epsilon}_1, \hat{\epsilon}_2, \hat{\epsilon}_3 \) and \( \hat{\epsilon}_4 \). The computation of Roe’s numerical flux (4.14), and subsequently, \( C_i^{n-1} \) in (4.5) is now straightforward.

5 The Numerical Computation of Strong or CJ Detonation Waves

In this section we want to compute strong or CJ detonation waves propagating with a constant wave speed \( s > 0 \), as described in Section 3. Let \( x_u, x_b \in \mathbb{R} \) be such that \( x_b < x_u \). The initial data \( u^0(x) \) are assumed to satisfy the following two conditions:

\[
u^0(x) = \begin{cases} u_b, & x \leq x_b, \\ u_u, & x \geq x_u, \end{cases} \tag{5.1a}
\]

i.e. the initial data are constant outside some finite interval. Physically (5.1a) and (5.1b) imply that at time \( t = 0 \) only burnt gas is present at the left-hand side of \( x_b \) and only unburnt gas is present at the right-hand side of \( x_u \).

In the remainder it is assumed that the exact solution of (2.2a) with initial data (2.2b) that satisfy (5.1) is a strong or CJ detonation wave propagating with a constant wave speed \( s > 0 \).

Let \([x_L, x_R] \subset \mathbb{R}\) be a fixed spatial interval. We want to approximate the numerical solution of (3.1) on \([x_L, x_R]\). Therefore, let \([x_L, x_R]\) be divided in a finite number of mesh cells, say \( I \). Hence, the mesh width \( \Delta x \) is defined by \((x_R - x_L)/I\). From (5.1) it immediately follows that we should take \( x_L < x_b < x_u < x_R \).
When attempting to solve (2.2) numerically, it is possible to obtain stable numerical solutions that seem reasonable and yet are completely wrong, since the reaction zone has the wrong location [6]. Thus the numerical combustion wave is propagating at non-physical wave speeds. In order to study this problem we consider numerical travelling wave solutions of (4.10) applied to the reactive Euler equations. We start with the introduction of the numerical wave speed and numerical combustion wave solutions.

Normally the numerical wave speed for a finite difference method is given by an expression of the form \( m \Delta x / (l \Delta t) \), where \( l \) and \( m \) are relatively prime numbers [9]. In other words, the numerical solution propagates \( m \) spatial grid points for every \( l \) time steps. In general it is hard to compute the numerical wave speed in this way. Using the behaviour of the exact solution we define a more general numerical wave speed which is easy to compute [2].

**Definition 5.1** Consider the finite difference method (4.10). Let \( U^n_i \) be a solution of (4.10) with given initial values \( U^0_i = u^0_i \), as defined in (4.3), that satisfy (5.1). Let \( T > 0 \) be given and assume that for all \( n > 0 \) with \( n \Delta t \leq T \) the following holds:

\[
\begin{align*}
U^n_i &= u^n_i = \hat{u}^0_i = u_b, \quad (5.2a) \\
U^n_{i+1} &= u^n_{i+1} = \hat{u}^0_{i+1} = u_u. \quad (5.2b)
\end{align*}
\]

If for all \( n > 0 \) with \( n \Delta t \leq T \) there exists a positive constant \( S^n \) such that

\[
S^n \Delta t (u_b - u_u) = \Delta x \left( \sum_{i=1}^{l} U^n_i - \sum_{i=1}^{l} U^{n-1}_i \right), \quad (5.3)
\]

then \( S^n \) is called the numerical wave speed at time level \( t^n \). If \( S^n \) is constant for all \( n > 0 \) with \( n \Delta t \leq T \), then \( U \) is called a numerical combustion wave solution.

Suppose the finite difference method produces a numerical solution that propagates with a speed given by \( m \Delta x / (l \Delta t) \). It follows that \( U^n_i = U^{n-1}_{i-m} \) for all \( n \) with \( 0 \leq l \Delta t \leq n \Delta t \leq T \) and \( x_L \leq x_L + m \Delta x \leq x_L + i \Delta x \leq x_R \). From (5.2) and (5.3) it follows that \( m \Delta x / (l \Delta t) = (S^n + S^{n-1} + \ldots + S^{n-l+1}) / l \). This illustrates that it is reasonable to define the numerical wave speed by (5.3).

**Theorem 5.2** Suppose that the finite difference method (4.10) is used to approximate the reactive Euler equations (3.1) with initial data that satisfy (5.1). Let \( U^n_i \) be a solution of (4.10) with given initial values \( U^0_i = \hat{u}^0_i \), as defined in (4.3). Let \( T > 0 \) be given and suppose that for all \( n > 0 \) with \( n \Delta t \leq T \) (5.2) holds, \( F^n_{1/2} = f(u_b) \) and \( F^n_{l+1/2} = f(u_u) \). If \( U \) is a numerical combustion wave solution propagating with a constant wave speed \( S \), then \( S \) satisfies the reactive Rankine-Hugoniot equations, i.e. the first three equations of (3.12).

**Proof** After multiplying (4.10) by \( \Delta x \) and summing over \( i \) we obtain

\[
\Delta x \left( \sum_{i=1}^{l} U^n_i - \sum_{i=1}^{l} U^{n-1}_i \right) = \Delta t \left( F^n_{1/2} - F^n_{l+1/2} \right) + \Delta x \sum_{i=1}^{l} q(U^n_i).
\]

Using (5.3), \( F^n_{1/2} = f(u_b) \) and \( F^n_{l+1/2} = f(u_u) \), we see that

\[
S \Delta t (u_b - u_u) = \Delta t \left( f(u_b) - f(u_u) \right) + \Delta x \sum_{i=1}^{l} q(U^n_i).
\]
Note that the first three equations are independent of \( q(U_i^0) \) and satisfy (3.12). This completes the proof.

**Theorem 5.3** Suppose that the finite difference method (4.10) is used to approximate the reactive Euler equations (3.1) with initial data that satisfy (5.1). Let \( U_i^0 \) be a solution of (4.10) with given initial values \( U_i^0 = U_i^0 \), as defined in (4.3). Suppose that (4.10) has a travelling combustion wave solution propagating with a constant numerical wave speed \( S > 0 \). Then,

(i) the numerical wave speed \( S \) is equal to the exact wave speed \( s \),

or,

(ii) the numerical travelling combustion wave solution is a weak detonation wave propagating with a numerical wave speed \( S > s \).

**Proof** Note that the form of the reaction rate \( \rho' \) in (3.4), implies that the reaction has to be initiated by an ordinary non-reacting shock wave, in order to raise the temperature above the ignition temperature. Since we assume that the first step of the splitting method consists of an entropy stable method, the non-reacting shock wave satisfies the entropy condition. Hence, the gas flow is supersonic relative to the shock, and therefore the shock has to be the front of a detonation wave (cf. Jouguet's rule).

Suppose that \( S \leq s \). It follows from \( u_i + e_u < S \) and \( s \leq u_i + e_u \) that \( u_i + e_u < S \leq u_i + e_u \). These inequalities together with \( S > u_i \) assert that one characteristic impinges the reaction zone from the left and three from the right, a total of four. This, together with the first three equations of (3.12), \( Y_i = 0 \) and \( Y_u = 1 \), gives seven equations for the seven variables \( u_i, u_u \) and \( S \). Since, by assumption \( (u_i, u_u, s) \) is the unique solution of this system of equations we find that \( S = s \).

Suppose that \( S > s \). If \( S \leq u_i + e_u \), then similar arguments show that \( S = s \). If \( S > u_i + e_u \), then the gas relative to the reaction front is supersonic behind the reaction front. Jouguet's rule implies that the combustion wave has to be a weak detonation wave. This completes the proof.

6 Numerical Results

In this section numerical results are presented for Roe's method, as described in Section 4.2. A natural choice for the initial data is \( u^0(x) = \overline{u} \) if \( x < 0 \) and \( u^0(x) = \underline{u} \) if \( x > 0 \). If Roe's method is applied to the reactive Euler equations with the previous initial data, then after some period a ZND-profile is formed. The numerical solution is then propagating with a constant numerical wave speed \( S \). However, our main goal in this paper is to study the behaviour of the numerical wave speed and not the formation of a ZND-profile. Therefore, we use in all our numerical examples initial data corresponding to the exact ZND-solution of a strong or CJ detonation, linking the states \( \overline{u} \) and \( \underline{u} \). Moreover, with these initial data we can compute the exact solution of the reactive Euler equations (3.1) easily, namely: \( u(x, t) = \overline{u}(x - st) \), where \( s \) is the exact wave speed of the detonation wave. This implies that we are able to compare the numerical results with the exact solution. It is assumed that at time \( t = 0 \) the precursor non-reacting shock wave is located at \( x = 0 \).
Example 6.1 In this example we approximate the ZND-solution of a strong detonation. Initially the dimensionless preshock state is given by

\[ p_u = 1, \quad \rho_u = 1, \quad u_u = 0. \]

Furthermore, we have the following parameter values:

\[ E_a = 10, \quad Q = 10, \quad f = 1.1, \quad \gamma = 1.4. \]

It can be shown that the corresponding burnt state of the exact ZND-solution is given by

\[ p_b = 13.481, \quad \rho_b = 2.0741, \quad u_b = 2.5423. \]

The exact propagation speed of this strong detonation is \( s = 4.9093 \) and the von Neumann pressure is \( p_{v,N} = 19.918 \).

Figure 2: Exact solution (dashed line) and numerical solution (solid line) at \( t = 20 \) of a strong detonation with \( E_a = 10, \quad Q = 10, \quad f = 1.1, \quad \gamma = 1.4, \quad T_{ign} = 1.01, \quad Da = 0.3310 \) (2 pts/L1/2), \( \Delta t = 0.1 \) and \( \Delta x = 1 \).

In Figure 2 the numerical results are compared with the exact solution. The Damkohler number \( Da \) is chosen such that \( L_{1/2} = 2 \) and, subsequently, since \( \Delta x = 1 \), there are two points per half-reaction length. Although the pressure peak is smeared out due to numerical diffusion, the numerical ZND-profile is essentially correct and the numerical wave speed is close to the exact wave speed.

Next we increase the Damkohler number such that \( L_{1/2} = 0.1 \). Since the wave speed is independent of \( Da \), the exact ZND-solution should still propagate with a wave speed \( s = 4.9093 \). However, Figure 3 clearly illustrates that the numerical solution is completely wrong. As predicted by Theorem 5.3, there is a weak detonation wave propagating with a numerical wave speed \( S = 10 > s \). In this weak detonation wave all energy is released and the gas is completely burnt. This phenomenon has been observed by several other authors [3, 6, 9, 12]. The weak detonation is a purely numerical artifact, since it disappears as the mesh is refined [6].

In order to explain the results in Figure 2 and 3 we have to study the behaviour of the numerical wave speed as the Damkohler number is increased (or as the number of points per half-reaction length is decreased). Note that increasing the Damkohler number only implies that the reaction becomes faster (i.e. the reaction time is decreased). The equilibrium
Figure 3: Exact solution (dashed line) and numerical solution (solid line) at $t = 20$ of a strong detonation with $E_a = 10$, $Q = 10$, $f = 1.1$, $\gamma = 1.4$, $T_{ign} = 1.01$, $Da = 6.6201$ (0.1 pts/$L_{1/2}$), $\Delta t = 0.1$ and $\Delta x = 1$.

conditions in front and behind the detonation wave and the speed of the detonation wave are not influenced by $Da$.

The results in Table 1 show that if the Dahmköhler number increases, then the relative error $|S - s|/|s|$ increases. Therefore, $Du$ influences the numerical solution in a similar way as the mesh size $\Delta x$, namely the results get better as $Da$ (or $\Delta x$) decreases. Obviously, the maximal numerical wave speed is equal to 10, since $S \Delta t / \Delta x \leq 1$ should hold.

| pts/$L_{1/2}$ | $Da$   | $S$            | $\frac{|S - s|}{s}$  |
|---------------|--------|----------------|----------------------|
| 5.0           | 0.1324 | 4.9096         | 0.5608 $\cdot 10^{-4}$ |
| 4.0           | 0.1655 | 4.9092         | 0.3242 $\cdot 10^{-4}$ |
| 3.0           | 0.2207 | 4.9763         | 0.1363 $\cdot 10^{-1}$ |
| 2.0           | 0.3310 | 4.9886         | 0.1614 $\cdot 10^{-1}$ |
| 1.5           | 0.4413 | 6.6662         | 0.3579 $\cdot 10^{+0}$ |
| 1.2           | 0.5517 | 7.5000         | 0.5277 $\cdot 10^{+0}$ |
| 1.0           | 0.6620 | 10.0000        | 0.1037 $\cdot 10^{+1}$ |
| 0.5           | 1.3240 | 10.0000        | 0.1037 $\cdot 10^{+1}$ |
| 0.1           | 6.6201 | 10.0000        | 0.1037 $\cdot 10^{+1}$ |

Table 1: Numerical results at $t = 200$ with $E_a = 10$, $Q = 10$, $f = 1.1$, $\gamma = 1.4$, $T_{ign} = 1.01$, $\Delta t = 0.1$ and $\Delta x = 1$.

The basic explanation for the occurrence of non-physical wave speeds is that the numerical propagation of the precursor shock wave results in a smeared representation of this shock wave, which includes intermediate temperatures $T_{n} \leq T \leq T_{b}$ in front of it. If the ignition temperature is close to $T_{n}$, then, due to numerical diffusion, the temperature is raised above the ignition temperature and an artificial reaction is started in front of the shock wave. If $Da$ is large enough, then the gas is completely burnt in the next time-step $\Delta t$ and the discontinuity is shifted to a cell boundary. Therefore, it is not surprising that non-physical wave speeds of one cell per time-step can be observed for large $Da$ [3, 6].
In practice the ignition temperature is much higher than $T_v$. For instance, when we consider the ZND-solution of detonation waves, it is realistic to choose the ignition temperature equal to the von Neumann temperature, since the ZND-theory assumes that no reaction takes place for all temperatures less than the von Neumann temperature $T_{vN}$. By choosing the ignition temperature just above $T_v$, the problem is made highly sensitive to numerical diffusion. The numerical diffusion in front of the non-reacting shock wave will cause a considerable increase of the numerical wave speed.

It seems that the ignition temperature plays a crucial role and therefore we have to study the influence of the ignition temperature on the numerical wave speed. Naturally, we restrict ourselves to very fast reactions, since in these cases the wrong wave speeds occur.

Example 6.2 In this example we consider the same strong detonation as in Example 6.1. In Figure 4 the numerical results are compared to the exact solution. Although there is some noise in the pressure behind the shock wave, we see a large improvement of the results compared to Figure 3 (where $T_{ign} = 1.01$). The disturbances behind the shock wave are caused by the splitting method. This will be explained later.

![Figure 4](image)

Figure 4: Exact solution (dashed line) and numerical solution (solid line) at $t = 20$ of a strong detonation with $E_a = 10$, $Q = 10$, $f = 1.1$, $\gamma = 1.4$, $T_{ign} = T_{vN}$, $Da = 6.6201$ (0.1 pts/$L_{1/2}$), $\Delta t = 0.1$ and $\Delta x = 1$.

The question is how the numerical solution, and especially the numerical wave speed, behaves if $T_{ign} < T_{vN}$. It is not a desirable situation if the method only produces the correct wave speed for one particular ignition temperature.

| $T_{ign}$ | $S$   | $\left| \frac{S - s}{s} \right|$ |
|-----|-----|-----------------|
| 1.0 | 10.000 | $0.1037 \cdot 10^{-1}$ |
| 2.0 | 5.0000 | $0.1847 \cdot 10^{-1}$ |
| 3.0 | 4.9064 | $0.6074 \cdot 10^{-3}$ |
| 4.0 | 4.9053 | $0.8208 \cdot 10^{-3}$ |
| $T_{vN}$ | 4.9070 | $0.4683 \cdot 10^{-3}$ |

Table 2: Numerical results at $t = 200$ with $E_a = 10$, $Q = 10$, $f = 1.1$, $\gamma = 1.4$, $Da = 6.6201$ (0.1 pts/$L_{1/2}$), $\Delta x = 1$, $\Delta t = 0.1$.  

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The results in Table 2 show that this is not the case. Only for ignition temperatures close to \( T_{\text{ign}} \approx 1 \), we observe the non-physical wave speeds. If \( T_{\text{ign}} \geq 3 \), then the numerical wave speed approximates the exact wave speed \( s = 4.9093 \) very well. Other authors have used a shock tracking method to derive the correct wave speed [3, 15]. Numerical computations show that these shock tracking methods produce similar wave speeds as the results in Table 2.

The disturbances in the numerical solution behind the reacting shock wave are caused by a combination of the Godunov-type method and the splitting method. For convenience sake we consider the basic Godunov method [1]. Consider the Riemann problem at the boundary of two adjacent cells separating the constant states \( u_b \) and \( u_w \). In the first step we derive the solution (or an approximation of the solution) of the Riemann problem at the cell boundary. Suppose that the solution consists of a simple wave, a contact discontinuity and a shock wave, respectively (see Figure 5). Note that for Roe's method shock waves and simple waves are replaced by contact discontinuities. For the sake of simplicity we restrict ourselves to the pressure. After the first step the pressure is equal to \( p_A = p_b \) in region \( A \), \( p_B \) in region \( B \), \( p_C \) in region \( C \) and \( p_D = p_w \) in region \( D \), where \( p_A > p_B = p_C > p_D \). Since region \( B \) and \( C \) are separated by a contact discontinuity, \( Y = 0 \) in \( B \) and \( Y = 1 \) in \( C \). In the second step, the gas is burnt in region \( C \) and, subsequently the pressure jumps to a higher value in this region. Since the pressure in region \( B \) remains the same in the second step (there is only burnt gas), \( p_C > p_B \). Hence, it is obvious that we observe oscillation in the numerical pressure behind the reacting shock wave. These oscillations will occur for all Godunov-type methods in combination with a splitting method. In order to avoid these oscillations it is necessary to know the position of the front accurately. One possibility is to use a front tracking method. Front tracking methods have been applied to the reactive Euler equations successfully by several authors [4, 3, 15].

Figure 5: Explanation of disturbances in the numerical solution behind the reacting shock wave.

**Example 6.3** We consider the ZND-solution of a CJ detonation as discussed in Example 3.1. All quantities are the same as in Example 3.1, except for the Dahmköhler number. In this example we consider a very fast reaction. The Dahmköhler number is given by \( Da = 6.4480 \cdot 10^{-3} \) (which implies that \( L_{1/2} = 10^{-4} \)). Note that we have to use a very fine mesh, if we want to represent the chemical reaction accurately. We use a relatively large mesh width \( \Delta x = 1 \). The initial data correspond to the exact CJ detonation.

In Figure 6 the numerical results are compared to the exact solution. The shock is almost at the correct location. The small error in the location of the shock is caused by some initiation process to start the numerical detonation wave. This error does not grow noticeably in time.
As expected we observe some noise behind the pressure peak. Due to the large mesh size, the pressure peak is smeared over two or three mesh points.

In Table 3 the numerical wave speed is shown for different values of $T_{\text{ign}}$. Similar to the results in Table 2 we see that if the ignition temperature is large enough, the numerical wave speed $S$ approximates the exact wave speed $s = 5.4419$ very well.

### Table 3: Numerical results at $t = 200$ with $E_a = 14$, $Q = 14$, $f = 1.0$, $\gamma = 1.4$, $T_{\text{ign}} = T_{\text{vN}}$, $Da = 6.488 \cdot 10^3$ ($10^{-4}$ pts/1/2), $\Delta t = 0.1$ and $\Delta x = 1$.  

| $T_{\text{ign}}$ | $S$       | $\left| \frac{S - s}{s} \right|$ |
|------------------|-----------|----------------------------------|
| 1.0              | 10.000    | 0.8376 $\cdot 10^{-1}$          |
| 2.0              | 6.9221    | 0.2720 $\cdot 10^{0}$           |
| 3.0              | 5.5567    | 0.2110 $\cdot 10^{-1}$          |
| 4.0              | 5.4399    | 0.3624 $\cdot 10^{-3}$          |
| 5.0              | 5.4275    | 0.2640 $\cdot 10^{-2}$          |
| $T_{\text{vN}}$  | 5.4396    | 0.4104 $\cdot 10^{-3}$          |

Table 3: Numerical results at $t = 200$ with $E_a = 14$, $Q = 14$, $f = 1.0$, $\gamma = 1.4$, $Da = 6.488 \cdot 10^3$ ($10^{-4}$ pts/1/2), $\Delta t = 0.1$ and $\Delta x = 1$.

Next we try to explain the good behaviour of the numerical method for high ignition temperatures. Suppose that we have a numerical travelling weak detonation wave propagating with a numerical wave speed $S > s$. Denote the burnt gas state behind this weak detonation wave by $\nu_b$. The state $\nu_b$ is linked to the given final state $\nu_b$ by the solution of the Riemann problem for the ordinary Euler equations. It is well known that this solution consists of constant states separated by shock waves, simple waves and/or contact discontinuities [10, 16]. Using the initial data $\nu_b$ and $\nu_b$ it can be shown that from right to left the solution of the Riemann problem consists of a shock wave, a contact discontinuity and a simple wave, respectively. We observed this solution earlier in Figure 3. Let the shock wave propagate with a constant speed $S_c > 0$ (see Figure 7). It is obvious that the above solution only exists if $S \geq S_c$. Hence, for each numerical weak detonation wave, there exists a minimum propagation speed, say $S_{\text{min}}$ [13]. It follows from numerical experiments that there exists a temperature $T_0$ with $T_u \leq T_0 \leq T_b$, such that no travelling combustion wave exists if $T_{\text{ign}} > T_0$. Let $T^-$ denote this
value corresponding to the weak detonation propagating with a speed $S_{\text{min}}$ and let $T^+$ denote this value corresponding to the desired strong or CJ detonation. If $T^- < T_{\text{ign}} < T^+$, then no weak detonation is possible and, subsequently, the numerical combustion wave is propagating with the correct speed. From numerical computations it follows that in practice obviously $T^- << T^+ \approx T_{\text{vN}}$.

![Schematic diagram of the numerical solution.](image)

Figure 7: Schematic diagram of the numerical solution.

References


