The one-dimensional reactive Euler equations

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Euler Equations
by
A.C. Berkenbosch
E.F. Kaasschieter
J.H.M. ten Thije Boonkkamp
The One-Dimensional Reactive Euler Equations

A.C. Berkenbosch, E.F. Kaasschieter and J.H.M. ten Thije Boonkkamp

Eindhoven University of Technology, Department of Mathematics and Computing Science, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.

Abstract

In this paper the reactive Euler equations are derived from the general conservation equations for reacting gas flow. We concentrate on travelling wave solutions of the reactive Euler equations. The Rankine-Hugoniot equations are presented, which relate the upstream and downstream conditions of combustion waves. A classification of combustion waves, based on the Rankine-Hugoniot equations, is given. Finally, the ZND-model is presented and detonation waves are described in more detail.

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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 [7, 9, 10, 11].

The basis for combustion theory are the conservation equations for reacting gas flow, together with chemical kinetics [9, 11]. These equations represent the conservation of mass, momentum and energy of the mixture as a whole and the conservation of mass for the various species. The general system of combustion equations describes a large class of combustion problems, but is generally quite complex. However, a considerable simplification of these equations is possible when we restrict ourselves to one-dimensional detonations. In this case the conservation equations reduce to the so-called reactive Euler equations [7, 9].

In this paper we adopt the general system of equations modelling a one-dimensional reacting gas flow and describe the assumptions that are made in order to derive the reactive Euler equations. Next we consider the ZND-model, which describes the travelling wave solution of the reactive Euler equations [7, 9]. In the derivation of the ZND-model, the well-known Rankine-Hugoniot equations play an important role. These equations link the upstream and downstream conditions of travelling combustion waves.

This paper is organized as follows. In the next section we present the physical set-up of the problem and adopt the conservation equations for reacting gas flow. In Section 3 the assumptions are described, which have to be made in order to derive the reactive Euler equations. In Section 4, the dimensionless equations are derived. The Rankine-Hugoniot equations are given in Section 5. Furthermore, in this section the Hugoniot curve is introduced. This curve is used to distinguish the several types of possible combustion waves. Finally, in Section 6 the ZND-model is described and equations are presented, that completely describe the solution of the reactive Euler equations in case of a detonation wave.

2 The One-Dimensional Conservation Equations for Reacting Gas Flow

Consider a tube filled with a gas mixture consisting of $N$ different chemical species, denoted by $M_i$ ($i = 1, 2, \ldots, N$), in which $M$ chemical reactions take place. We assume the existence of $N$ distinct continua in any control volume, corresponding with the $N$ chemical species, and each continuum obeys the laws of dynamics and thermodynamics.

Suppose that the gas mixture is uniform across the tube, so there is variation only in one direction and we can restrict ourselves to one space dimension. Further assume that a combustion wave is propagating in the positive $x$-direction. This combustion wave consists of a zone involving chemical reactions, heat conduction, mass diffusion and viscous effects. Ahead of the combustion wave there is a mixture of reactants that are in equilibrium. In the combustion wave the gas is burning and all reactants are entirely converted into products such that at the end of the zone the mixture consists of products only. Conditions ahead of the combustion wave will be identified by the subscript $u$ (the unburnt gas), while conditions behind the wave are denoted by the subscript $b$ (the burnt gas).

For this kind of combustion problems, chemical reactions between the constituent gases need to be modelled together with the fluid dynamics. Therefore, we consider the conservation equations for reacting gas flow. These equations represent the conservation of mass, momentum and energy of the mixture as a whole and the conservation of mass for the various
Zone involving reaction, heat conduction, mass diffusion and viscous effects

\[
\begin{align*}
\rho_b & \quad \rho_b \\
u_b & \quad E_b \\
Y_{i,b} & \quad T_b \\
\rho_u & \quad \rho_u \\
u_u & \quad E_u \\
Y_{i,u} & \quad T_u
\end{align*}
\]

Figure 1: Schematic diagram of the tube.

species. The latter equations include source terms which describe the chemical reactions that take place.

In this paper we adopt the equations modelling a reacting gas flow. For details of the derivation of these equations the reader is referred to e.g. [9, 11]. With mass density \( \rho \), mass-weighted average velocity \( u \), mass fractions \( Y_j \), reaction rates \( w_i \), stress \( \sigma \), external forces \( f_i \), specific total energy \( E \) and heat flux \( q \) the one-dimensional conservation equations for reactive gas flow are [9, 10, 11]

\[
\begin{align*}
\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) &= 0, \quad (2.1a) \\
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) &= \frac{\partial}{\partial x}(\sigma) + \rho \sum_{j=1}^{N} Y_j f_j, \quad (2.1b) \\
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x}(\rho u E) &= -\frac{\partial}{\partial x}(\sigma u) + \rho \sum_{j=1}^{N} Y_j f_j (u + U_j), \quad (2.1c) \\
\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x}(\rho u Y_i) &= -\frac{\partial}{\partial x}(\rho Y_i U_i) + w_i, \quad i = 1, 2, \ldots, N. \quad (2.1d)
\end{align*}
\]

The reaction rate \( w_i \) is defined as the mass of species \( M_i \) created or destroyed by chemical reactions, per unit volume and per unit time. Since total mass is neither created nor destroyed by chemical reactions, it is obvious that

\[
\sum_{j=1}^{N} w_j = 0. \quad (2.2)
\]

The mass fraction \( Y_i \) of species \( M_i \) is given by \( Y_i := \rho_i / \rho \), where \( \rho_i \) denotes the mass density of species \( M_i \). Evidently, the mass fractions satisfy

\[
\sum_{j=1}^{N} Y_j = 1. \quad (2.3)
\]

It is customary to write the flow velocity \( u_i \) of species \( M_i \) as

\[
u_i = u + U_i, \quad (2.4a) \]
where the mass-weighted average velocity $u$ is given by

$$u := \sum_{j=1}^{N} Y_{j} u_{j}.$$  

(2.4b)

Using the above equations it can be easily shown that

$$\sum_{j=1}^{N} Y_{j} U_{j} = 0.$$  

(2.5)

The set of equations (2.1) has to be completed with models for $U_{i}$, $W_{i}$, $\sigma$, $f_{i}$ and $q$. A brief description of these physical/chemical parameters follows in the next section; for more details the reader is referred to [9, 11].

System (2.1) describes a large class of combustion problems, but is generally quite complex. Therefore, in the next section several assumptions are made in order to simplify (2.1) considerably.

3 Derivation of the One-Dimensional Reactive Euler Equations

In this section the reactive Euler equations will be derived. We start with the general system of equations (2.1) and list the assumptions to simplify (2.1) and to derive the reactive Euler equations.

We start with the following two assumptions [10, 11].

**A1** *The external forces $f_{i}$ are negligible.*

**A2** *The mass diffusion caused by pressure and thermal gradients (known as the Soret effect) is negligible.*

Under the assumptions A1 and A2 the diffusion velocities $U_{i}$ can be determined from the *Stephan-Maxwell equations* [9, 11]

$$\frac{\partial}{\partial x} X_{i} = \sum_{j=1}^{N} \frac{X_{i} X_{j}}{D_{ij}} (U_{j} - U_{i}), \quad i = 1, 2, \ldots, N,$$

(3.1)

where $D_{ij}$ is the *binary diffusion coefficient* for species $M_{i}$ and $M_{j}$. The variable $X_{i}$ is the *mole fraction* of species $M_{i}$, and is related to the mass fraction $Y_{i}$ by

$$X_{i} = \frac{WY_{i}}{W_{i}}, \quad i = 1, 2, \ldots, N,$$

(3.2a)

where $W_{i}$ is the *molecular weight* of species $M_{i}$ and $W$ is the *average molecular weight* of the gas mixture, defined by

$$W := \sum_{j=1}^{N} X_{j} W_{j}.$$  

(3.2b)

Equation (3.1) can be simplified considerably if the following assumption is made.

**A3** *All binary diffusion coefficients are equal, i.e. $D_{ij} = D$ for all $i$ and $j$.***
From (2.3), (2.5), (3.1), (3.2) and assumption A3, Fick's law of mass diffusion follows, i.e.

\[ Y_i U_i = -D \frac{\partial}{\partial x} Y_i, \]  

(3.3)

Concerning the stress \( \sigma \) the following is assumed [10, 11].

**A4** The mixture behaves like a Newtonian fluid for which the bulk viscosity can be neglected.

Then \( \sigma \) can be written as

\[ \sigma = -p + \tau, \]  

(3.4)

where \( p \) is the hydrostatic pressure and \( \tau \) is the viscous stress. According to assumption A4, \( \tau \) is defined by

\[ \tau := \frac{4}{3} \mu \frac{\partial}{\partial x} u, \]  

(3.5)

where \( \mu \) is the viscosity of the gas mixture. In general \( \mu \) is a function of the temperature, the pressure and the mole fractions. Using (3.4) and (3.5), the stress terms in the momentum equation and in the energy equation can be reduced to

\[
\begin{align*}
\frac{\partial}{\partial x} \sigma &= -\frac{\partial}{\partial x} p + 4 \frac{\partial}{\partial x} (\mu \frac{\partial}{\partial x} u), \\
\frac{\partial}{\partial x} (\sigma u) &= -\frac{\partial}{\partial x} (pu) + 4 \frac{\partial}{\partial x} (\mu u \frac{\partial}{\partial x} u).
\end{align*}
\]

(3.6a) \hspace{1cm} (3.6b)

In many applications the following assumption is justified [11].

**A5** The viscous term \( \frac{\partial}{\partial x} (\mu \frac{\partial}{\partial x} u) \) in the energy equation is negligible.

This assumption implies that (3.6b) simplifies to

\[ \frac{\partial}{\partial x} (\sigma u) = -\frac{\partial}{\partial x} (pu). \]  

(3.6c)

In order to describe the heat flux \( q \) of the mixture we assume the following [11].

**A6** Heat transfer caused by radiation and concentration gradients (known as the Dufour effect) are negligible.

This implies that the heat flux \( q \) of the gas mixture is given by [9, 11]

\[ q = -\lambda \frac{\partial}{\partial x} T + \rho \sum_{j=1}^{N} h_j Y_j U_j, \]  

(3.7)

where \( T \) is the absolute temperature of the gas mixture, \( \lambda \) is the thermal conductivity of the gas mixture and \( h_i \) is the specific enthalpy of species \( M_i \), which is defined by the caloric equation of state

\[ h_i := h_i^0 + \int_{T_0}^{T} c_{p,i}(\xi) d\xi, \quad i = 1, 2, \ldots, N. \]  

(3.8)

The parameter \( h_i^0 \) is the standard heat of formation per unit mass for species \( M_i \) at a reference temperature \( T_0 \), and \( c_{p,i} = c_{p,i}(T) \) is the specific heat at constant pressure for species \( M_i \).
After substituting the above models into (2.1) we derive the following set of equations for a reacting gas flow:

\[ \frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) = 0, \]  

(3.9a)

\[ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) = \frac{4}{3} \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}), \]  

(3.9b)

\[ \frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x}(\rho u E + pu) = \frac{\partial}{\partial x}(\lambda \frac{\partial T}{\partial x}) + \frac{\partial}{\partial x}(\rho D \sum_{j=1}^{N} h_j \frac{\partial Y_j}{\partial x}), \]  

(3.9c)

\[ \frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x}(\rho u Y_i) = \frac{\partial}{\partial x}(\rho D \frac{\partial Y_i}{\partial x}) + w_i, \quad i = 1, 2, \ldots, N. \]  

(3.9d)

System (3.9) consists of \( N + 3 \) equations, however it follows from (2.2) and (2.3) that (3.9a) is the sum of (3.9d) for the individual species. Therefore, only \( N + 2 \) of these equations are independent. The independent variables are: \( \rho, u, N - 1 \) mass fractions \( Y_i, p, E \) and \( T \); thus we have \( N + 4 \) unknowns. Therefore, two extra equations are required to complete the system. These equations are the equation of state and the thermodynamic identity.

A7 The gas mixture behaves like an ideal gas.

Under this assumption the equation of state becomes

\[ p = \rho RT/W, \]  

(3.10a)

where \( R \) is the universal gas constant. Furthermore, the thermodynamic identity for an ideal gas is given by

\[ h := e + \frac{p}{\rho} = \sum_{j=1}^{N} Y_j h_j, \]  

(3.10b)

where \( h \) is the specific enthalpy of the mixture and \( e \) the specific internal energy. The specific internal energy \( e \) is related to the specific total energy \( E \) by the relation

\[ E = e + \frac{1}{2} u^2. \]  

(3.11)

The term \( u^2/2 \) in (3.11) represents the specific kinetic energy of the gas mixture. Equation (3.10b) defines \( e \) as a function of \( T \) and \( Y_i \) through the caloric equation of state (3.8) and the equation of state (3.10a).

Let the specific heat \( c_p \) at constant pressure for the gas mixture be defined as

\[ c_p(T) := \sum_{j=1}^{N} Y_j c_{p,j}(T). \]  

(3.12)

For a mixture behaving like an ideal gas the specific heat \( c_v \) at constant volume for the gas mixture is defined as

\[ c_v(T) := c_p(T) - \frac{R}{W}. \]  

(3.13)

In order to elaborate (3.10b) in more detail we make one more assumption \([10, 11]\).
A8 All chemical species have constant and equal specific heats $c_p$ at constant pressure.

Using (3.8), (3.10b) and assumption A8, we derive

$$h = \sum_{j=1}^{N} Y_j h_j^0 + c_p(T - T_0).$$  \hspace{1cm} (3.14)

Furthermore, we assume the following [10, 11].

A9 The gas is a binary mixture in which only one chemical reaction takes place.

Of course assumption A9 is often not true. However, the global chemical behaviour of a mixture can often be modelled quite adequately by a single reaction. Consider therefore, the one-step reaction in which a reactant $R$ is converted into a product $P$. Note that in this case $W = W_1 = W_2$ and let $Y_1 = Y$ denote the mass fraction of the reactant (and consequently $Y_2 = 1 - Y$). Since $N = 2$, we have $\sum_{j=1}^{2} h_j \frac{\partial}{\partial x} Y_j = (h_1 - h_2) \frac{\partial}{\partial x} Y$. Using assumptions A8 and A9, the heat release $Q$ of the reaction per unit mass is given by [9, 11]

$$Q = h_1^0 - h_2^0.$$  \hspace{1cm} (3.15)

Equation (3.14), together with assumptions A8 and A9, and (3.15) gives

$$h = Q Y + c_p T,$$  \hspace{1cm} (3.16)

where, for convenience sake, we assume that $h_2^0 = c_p T_0$. It follows from the latter equation, (3.10a), (3.11) and (3.13) that we can also write the thermodynamic identity (3.10b) as

$$p = (\gamma - 1) \rho (E - \frac{1}{2} u^2 - Q Y),$$  \hspace{1cm} (3.17)

where $\gamma = c_p/c_v$ is the specific heat ratio.

Until now we have not specified how the reaction rates $w_i$ depend on the other variables. Since $Y$ denotes the mass fraction of the reactant we write $w := w_1 = -w_2$ (see (2.2)). We assume that the one-step reaction is described by the law of mass action [10, 11]

$$w = -k \rho Y,$$ \hspace{1cm} (3.18a)

where $k$ is the specific rate constant for the reaction. We assume that $k$ satisfies Arrhenius' law

$$k = A(T) \exp\left(- \frac{E_a}{RT}\right),$$  \hspace{1cm} (3.18b)

$$A(T) = BT^\alpha.$$  \hspace{1cm} (3.18c)

The coefficients $A$ and $E_a$ in (3.18) are the frequency factor and the activation energy, respectively, for the reaction. Further $B$ is some positive fixed constant.

When we consider chemical reactions with very thin reaction zones, energy release occurs so quickly that molecular diffusion, thermal conductivity and viscosity are usually unimportant transport mechanisms. Furthermore, for this kind of reactions the temperature dependence of the frequency factor $A$ is rather unimportant. Therefore, for such reactions the following assumptions seem reasonable [6, 7, 9].

A10 The molecular diffusion, the thermal conductivity and the viscosity are negligible ($D = 0$, $\lambda = 0$ and $\mu = 0$).
The temperature dependence of the frequency factor in the reaction rate is negligible \((\alpha = 0, \text{thus } A(T) = A)\).

Using all the above results and assumptions in (3.9), we obtain the **reactive Euler equations** [2, 4, 7]

\[
\begin{align*}
\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) &= 0, \\
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) &= 0, \\
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x}(\rho u E + pu) &= 0, \\
\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial x}(\rho u Y) &= w.
\end{align*}
\]

The system of equations (3.10a), (3.17), (3.18) and (3.19) consists of 8 equations for the variables \(\rho, u, Y, p, E, T, k\) and \(w\).

This section is concluded by introducing two quantities which will be useful later on. Firstly, we define the **specific entropy** \(S\) for fixed \(Y\) by the second law of thermodynamics [5], i.e.

\[
TdS = dh - \frac{1}{\rho}dp.
\]

Finally, it will also be convenient to introduce the **frozen speed of sound** \(c\), which for an ideal gas is given by

\[
c = \sqrt{\frac{T \rho}{\mu}}.
\]

### 4 Dimensionless Equations

Often it is convenient to use dimensionless variables. In this section we want to derive the dimensionless formulation of the reactive Euler equations (3.19) together with the ideal gas law (3.10a), the thermodynamic identity (3.17) and the reaction rate (3.18).

Let \(\rho_{ref}, \rho_{ref}, u_{ref}, x_{ref}\) and \(t_{ref}\) be some given reference values of \(\rho, u, x, x\) and \(t\), respectively. We introduce the following dimensionless variables [7]

\[
\begin{align*}
\tilde{E} & := \frac{E}{u_{ref}^2}, \\
\tilde{p} & := \frac{p}{\rho_{ref}}, \\
\tilde{\rho} & := \frac{\rho}{\rho_{ref}}, \\
\tilde{t} & := \frac{t}{t_{ref}}, \\
\tilde{u} & := \frac{u}{u_{ref}}, \\
\tilde{w} & := \frac{w}{\rho_{ref}}, \\
\tilde{x} & := \frac{x}{x_{ref}}.
\end{align*}
\]

Note that the mass fraction \(Y\) is not scaled since it is dimensionless already. If we require that the following relations hold

\[
t_{ref} = \frac{x_{ref}}{u_{ref}}, \quad u_{ref} = \sqrt{\frac{p_{ref}}{\rho_{ref}}},
\]
then a straightforward substitution into (3.19) shows that the dimensionless Euler equations are given by

\[ \frac{\partial (\tilde{\rho})}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u})}{\partial x} = 0, \]

\[ \frac{\partial (\tilde{\rho} \tilde{u})}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}^2 + \tilde{p})}{\partial x} = 0, \]

\[ \frac{\partial (\tilde{\rho} \tilde{E})}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u} \tilde{E} + \tilde{p} \tilde{u})}{\partial x} = 0, \]

\[ \frac{\partial (\tilde{\rho} Y)}{\partial t} + \frac{\partial (\tilde{p} \tilde{Y})}{\partial x} = \tilde{w}. \]

Let the dimensionless activation energy \( \tilde{E}_a \), the dimensionless heat release of the chemical reaction \( \tilde{Q} \) and the dimensionless temperature \( \tilde{T} \) be introduced as

\[ \tilde{E}_a := E_a \frac{\rho_{ref}}{\rho'_{ref}}, \quad \tilde{Q} := Q \frac{\rho'_{ref}}{\rho_{ref}}, \quad \tilde{T} := T \frac{R \rho_{ref}}{W_{ref}}. \]

The dimensionless equation of state and the dimensionless thermodynamic identity are given by, respectively,

\[ \tilde{p} = \tilde{\rho} \tilde{T}, \]

\[ \tilde{p} = (\gamma - 1)\tilde{\rho}(\tilde{E} - \frac{1}{2} \tilde{u}^2 - \tilde{Q} Y). \]

Let \( k_{ref} \) be a typical specific rate constant (see (3.18b)) and suppose that the dimensionless rate constant \( \tilde{k} \) is defined as \( \tilde{k} := k / k_{ref} \). Using this, \( \tilde{\omega} = \tilde{w} t_{ref} / \rho_{ref} \) and (3.18a), the dimensionless reaction rate can be given by

\[ \tilde{\omega} = -D a \tilde{k} \tilde{\rho} Y, \]

where the dimensionless constant \( D a \) is defined by

\[ D a := t_{ref} k_{ref}. \]

The constant \( D a \) is referred to as the Damköhler number, although there are several Damköhler numbers [9]. Suppose \( x_{ref} \) is a typical length scale based on the convection of the flow, for instance the length of a finite tube (see Figure 1) in a laboratory. If \( u_{ref} \) is of the same order as the speed of the combustion wave, then \( u_{ref} / k_{ref} \) can be interpreted as a characteristic reaction length [6, 9]. It follows from (4.1) and (4.6) that the Damköhler number is the ratio of the convection length scale and the reaction length scale [9]. Obviously, if \( D a \) is small the reaction occurs slowly relative to the specified time scale and if \( D a \) is large, the reaction zone is thin and the reaction occurs quickly relative to the specified time scale \( t_{ref} \).

It will be useful to introduce the dimensionless specific enthalpy \( \tilde{h} \), the dimensionless specific entropy \( \tilde{S} \) and the dimensionless speed of sound \( \tilde{c} \) as

\[ \tilde{h} := h \frac{\rho_{ref}}{\rho'_{ref}}, \quad \tilde{S} := S \frac{W}{R}, \quad \tilde{c} := c \sqrt{\frac{\rho_{ref}}{\rho'_{ref}}}. \]

It follows directly from (3.13) and (3.16) that

\[ \tilde{h} = \tilde{Q} Y + \frac{\gamma}{\gamma - 1} \tilde{T}. \]
Also it is easy to see that (3.20) gives

\[ \tilde{T} d\tilde{S} = d\tilde{h} - \frac{1}{\tilde{\rho}} d\tilde{p}. \]  

(4.8)

Finally, one can easily verify that (3.21) implies

\[ \tilde{c} = \sqrt{\frac{\gamma \tilde{p}}{\tilde{\rho}}}. \]  

(4.9)

In the remainder it is assumed that all variables are dimensionless, where, for shortness of notation, the tilde is suppressed.

5 The Rankine-Hugoniot Equations

5.1 Derivation of the Rankine-Hugoniot Equations

As in Section 2, we assume that a combustion wave is propagating with a certain velocity \( s \) in the positive \( x \)-direction of the tube (the direction of the unburnt gas, see Figure 1). It is clear that \( s > u_u \) and \( s > u_b \), since otherwise the wave will never pass the unburnt gas. The main goal of this section is to derive equations that relate the state of the unreacted gas at the downstream side of the tube \( (x = +\infty) \) with the state of the completely reacted gas, at the upstream side of the tube \( (x = -\infty) \).

We make the following assumptions [5, 7, 11].

\( \text{A12} \) The flow is steady with respect to a coordinate system moving with the combustion wave \( (s > 0 \) is constant). \n
\( \text{A13} \) The chemical reaction is exothermic, i.e. \( Q > 0 \).

According to A12, it is natural to introduce a coordinate system which is stationary with respect to the wave. Therefore, the variable \( \xi \) is introduced as

\[ \xi(x, t) := x - st. \]  

(5.1)

Using (5.1) and assumption A12 we write \( g(x, t) = g(x - st) = g(\xi) \) for all variables \( g \). Subsequently, (4.2) can be rewritten as a system of ordinary differential equations, i.e.

\[ -s \frac{d}{d\xi} (\rho) + \frac{d}{d\xi} (\rho u) = 0, \]  

(5.2a)

\[ -s \frac{d}{d\xi} (\rho u) + \frac{d}{d\xi} (\rho u^2 + p) = 0, \]  

(5.2b)

\[ -s \frac{d}{d\xi} (\rho E) + \frac{d}{d\xi} (\rho u E + pu) = 0, \]  

(5.2c)

\[ -s \frac{d}{d\xi} (\rho Y) + \frac{d}{d\xi} (\rho u Y) = w. \]  

(5.2d)

Now we are able to obtain the Rankine-Hugoniot equations. After integrating (5.2a) from \( \xi = -\infty \) towards \( \xi = +\infty \), we deduce

\[ \rho_u (u_u - s) = \rho_b (u_b - s) = -m, \]  

(5.3a)
where \( m > 0 \) is the so-called dimensionless mass flux. Similarly, (5.2b) is integrated, which gives, using (5.3a),

\[
\rho_u (u_u - s)^2 + p_u = \rho_b (u_b - s)^2 + p_b. \tag{5.3b}
\]

Integrating (5.2c) implies \(-m E_u + p_u u_u = -m E_b + p_b u_b\). It follows from (4.3), (4.4) and (4.7) that \( h = E - \frac{u^2}{2} + p / \rho \). Using this together with (5.3a) and (5.3b) the latter equation can be rewritten as

\[
h_u + \frac{1}{2} (u_u - s)^2 = h_b + \frac{1}{2} (u_b - s)^2. \tag{5.3c}
\]

The equations (5.3) are called the Rankine-Hugoniot equations \([5, 7, 9, 11]\).

Integrating (5.2d) gives, using (5.3a), \( Y_u = 1 \) and \( Y_b = 0 \)

\[-m = \int_{-\infty}^{\infty} w(\xi) d\xi. \]

This provides the additional requirements

\[
w_u = w_b = 0. \tag{5.4}
\]

The equation of state (4.3)

\[
\frac{p_u}{\rho_u T_u} = \frac{p_b}{\rho_b T_b} \tag{5.5}
\]

and the thermodynamic relation (4.7)

\[
h_b - \frac{\gamma}{\gamma - 1} T_b = h_u - Q - \frac{\gamma}{\gamma - 1} T_u = 0 \tag{5.6}
\]

constitute further relations between the variables at \( \xi = -\infty \) and \( \xi = +\infty \).

The set of states at \( \xi = -\infty \) (with fixed parameters at \( \xi = +\infty \)) for which equations (5.3a) and (5.3b) are satisfied is often referred to as the Rayleigh line. It follows directly from (5.3a) and (5.3b) that the Rayleigh line is given by

\[
\frac{p_u - p_b}{(1 / \rho_u) - (1 / \rho_b)} = -m^2 < 0. \tag{5.7}
\]

Using equation (5.3a) to express \( u - s \) in terms of \( m \) and \( \rho \) in equation (5.3c) yields

\[
h_b - h_u = \frac{1}{2} \left( \frac{1}{\rho_b} + \frac{1}{\rho_u} \right) (p_b - p_u), \tag{5.8}
\]

where equation (5.7) is used to eliminate \( m^2 \). Since the velocities have been eliminated, the latter equation is a relationship among thermodynamic properties alone. In summary, equations (5.3), (5.5) and (5.6) complete the independent relations between the burnt and unburnt conditions. If all unburnt conditions (conditions at \( \xi = +\infty \)) are specified, then these 5 equations completely determine the variables \( u_b, \rho_b, p_b, T_b \) and \( h_b \).

5.2 The Hugoniot Curve

Suppose that all conditions in the unburnt gas are specified. We want to describe the set of possible conditions in the completely burnt gas, such that all relations given in the previous section are fulfilled. Therefore, the subscript \( b \) is suppressed and all burnt conditions are
considered to be variable. Since \( Y_b \) vanishes and \( Q \) is constant, (4.3) and (4.7) imply that the specific enthalpy \( h \) of the completely burnt gas can be expressed in terms of \( 1/\rho \) and \( p \), i.e. \( h = h(1/\rho, p) \). For shortness of notation, the specific volume \( v \) is introduced as

\[
v := 1/\rho.
\]

We define the Hugoniot function \( \mathcal{H} \) by

\[
\mathcal{H}(v, p) := h(v, p) - h_u - \frac{1}{2} (v + v_u)(p - p_u),
\]

where (4.7) implies \( h_u = Q + T_u \gamma / (\gamma - 1) \). It is straightforward to see that the equation \( \mathcal{H} = 0 \) defines a curve in \((v, p)\)-space. This curve is called the Hugoniot curve. It follows from \( Y_u = 1, Y_b = 0 \), (4.3) and (4.7) that

\[
h(v, p) - h_u = -Q + \frac{\gamma}{\gamma - 1} (pv - p_u v_u).
\]

After substituting the latter equation into (5.10) we obtain

\[
\mathcal{H}(v, p) = -Q + \frac{\gamma}{\gamma - 1} (pv - p_u v_u) - \frac{1}{2} (v + v_u)(p - p_u).
\]

One can easily verify that the Hugoniot curve \( \mathcal{H} = 0 \) can be written as

\[
p(v) = \frac{2Q - p_u v + \frac{\gamma + 1}{\gamma - 1} p_u v_u}{\frac{\gamma + 1}{\gamma - 1} v - v_u}.
\]

Furthermore, the Rayleigh line (5.7) is rewritten as

\[
p(v) = -m^2 (v - v_u) + p_u.
\]

The intersection of the Hugoniot curve with the Rayleigh line determines the final thermodynamic state, after \( m \) has been obtained from \( p_u, v_u \) and \( s \) for the particular experiment. The value \( v_u \) may then be calculated from (5.3a). In Figure 2 the Hugoniot curve (5.13) is drawn for \( \gamma = 1.4 \) and several values of the heat release \( Q \).

Since the pressure \( p \) and the specific volume \( v \) should be positive we require

\[
\frac{\gamma - 1}{\gamma + 1} v_u < v < \frac{2Q}{p_u} + \frac{\gamma + 1}{\gamma - 1} v_u,
\]

\[
0 < p < \infty,
\]

where the upper bound of \( v \) corresponds to the limit \( p \to 0 \).

### 5.3 Various Types of Processes.

The intersection between the Hugoniot curve and the Rayleigh line (5.14) determines the conditions in the burnt gas. Since \( m^2 > 0 \), the slope of the Rayleigh line is negative and end states lying in the two shaded regions in Figure 2 are physically meaningless. Each Hugoniot curve is therefore divided into two distinct branches. The upper branch, which is given by (5.13) with

\[
\frac{(\gamma - 1)Q}{v_u} + p_u \leq p < \infty,
\]

\[
\frac{\gamma - 1}{\gamma + 1} v_u < v \leq v_u,
\]
Figure 2: Hugoniot curves from (5.13) with \( v_u = p_u = 1 \) and \( \gamma = 1.4 \).

is called the *detonation branch*. The lower branch, which is given by (5.13) with

\[
0 < p \leq p_u, \\
v_u + \frac{Q(\gamma - 1)}{\gamma p_u} \leq v < \frac{2Q}{p_u} + \frac{\gamma + 1}{\gamma - 1} v_u,
\]

is called the *deflagration branch*. Acceptable states of the burnt gas must lie on one of these two branches. Combustion waves are termed detonation waves or deflagration waves according to the branch of the Hugoniot curve upon which the final condition falls.

It can be shown that there are at most two points of intersection between the Rayleigh line and the detonation branch of the Hugoniot curve. There is a unique slope of the Rayleigh line such that it is tangent to the detonation branch. This point of tangency (point \( B \) in Figure 3) separates the detonation branch in two parts and is called the *upper Chapman-Jouguet point* (upper CJ point). Any straight line through \((v_u, p_u)\) with a slope less than that of the line through \( B \) intersects the Hugoniot curve in two points (the steepest dashed line in Figure 3). Depending on the final conditions of the detonation we can distinguish three different processes [5, 7, 9].

(i) Detonation waves with final conditions on the line \( AB \) are called *strong detonations*.

(ii) Detonation waves with final conditions at point \( B \) are called *Chapman-Jouguet detonations* (CJ detonations).

(iii) Detonation waves with final conditions on the line \( BC \) are called *weak detonations*.

There is also a unique slope of the Rayleigh line, such that it is tangent to the deflagration branch of the Hugoniot curve. This point of tangency (point \( E \) in Figure 3) separates the
deflagration branch in two parts and is called the **lower Chapman-Jouguet point** (lower CJ point). Similarly to detonation waves we can distinguish three different deflagration waves [5, 7, 9].

(i) Deflagration waves with final conditions on the line $DE$ are called **weak deflagrations**.

(ii) Deflagration waves with final conditions at point $E$ are called **Chapman-Jouguet deflagrations** (CJ deflagrations).

(iii) Deflagration waves with final conditions on the line $EF$ are called **strong deflagrations**.

![Figure 3: Different sections of the Hugoniot curve (5.13).](image)

In the remainder we restrict ourselves to detonation waves. Next we elaborate the detonation processes in more detail [7, 9]. Let final conditions for a strong, Chapman-Jouguet and weak detonation be denoted by the subscripts $s$, $CJ$ or $w$, respectively. It follows from (5.13) and (5.14) that the mass-flux $m_{CJ} > 0$, is given by

$$m_{CJ}^2 = \gamma \frac{p_u}{v_u} + (\gamma^2 - 1) \frac{Q}{v_u^2} \left(1 + \sqrt{1 + \frac{2\gamma p_u v_u}{(\gamma^2 - 1)Q}}\right).$$

(5.15)

For all $m < m_{CJ}$ there will be no detonation. If $m = m_{CJ}$, then there will be a CJ detonation with final conditions

$$p_{CJ} = \frac{m^2 v_u + p_u}{\gamma + 1},$$

(5.16a)

$$v_{CJ} = \frac{\gamma (m^2 v_u + p_u)}{m^2 (\gamma + 1)},$$

(5.16b)

$$u_{CJ} = s_{CJ} - v_{CJ} m.$$  

(5.16c)
If \( m > m_{cJ} \), then there will be a detonation with final conditions

\[
\begin{align*}
\rho_s &= \frac{m^2 v_u + p_u}{\gamma + 1} + \frac{1}{\gamma + 1} \sqrt{(m^2 v_u - \gamma p_u)^2 - 2(\gamma^2 - 1)m^2 Q}, \\
v_s &= \frac{\gamma(m^2 v_u + p_u)}{m^2(\gamma + 1)} - \frac{1}{m^2(\gamma + 1)} \sqrt{(m^2 v_u - \gamma p_u)^2 - 2(\gamma^2 - 1)m^2 Q}, \\
u_s &= s_s - v_s m,
\end{align*}
\]

in case of a strong detonation and

\[
\begin{align*}
p_w &= \frac{m^2 v_u + p_u}{\gamma + 1} - \frac{1}{\gamma + 1} \sqrt{(m^2 v_u - \gamma p_u)^2 - 2(\gamma^2 - 1)m^2 Q}, \\
v_w &= \frac{\gamma(m^2 v_u + p_u)}{m^2(\gamma + 1)} + \frac{1}{m^2(\gamma + 1)} \sqrt{(m^2 v_u - \gamma p_u)^2 - 2(\gamma^2 - 1)m^2 Q}, \\
u_s &= s_w - v_w m,
\end{align*}
\]

in case of a weak detonation.

Finally, we present, without a proof, some characteristic properties by which we can distinguish the various detonation waves. These properties are referred to as Jouguet’s Rule [5]. Let \( c_u \) denote the speed of sound ahead of the reaction front and let \( c_b \) denote the speed of sound behind the reaction front.

**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. \( s - u_b > c_b \)).

### 6 The ZND-Model for Detonation Waves

The Rankine-Hugoniot equations give no insight into the internal structure of detonation waves. 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 [5, 7, 9]. Apart from the assumptions A1-A13 the ZND-model also assumes the following.

**A14** 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 reaction zone.

The shock wave is assumed to be much thinner than the zone of chemical reaction, thus the shock can be considered as a discontinuous jump. This assumption is physically reasonable, since a few collisions in the material will establish a mechanical equilibrium behind the shock, but many collisions are required for creating enough energy to initiate the chemical reaction [7, 9]. Hence, the front of a detonation wave is a shock wave that initiates a chemical reaction behind it. We assume the following.
A15 The reaction rate is zero ahead of the shock and finite behind.

A16 All thermodynamic variables of the gas mixture are in local thermodynamic equilibrium everywhere.

We still assume that effects of mass diffusion, thermal conductivity and viscosity are negligible (assumption A11) and that the flow is steady with respect to a coordinate system moving with the detonation wave (assumption A12). Assumption A16 implies that the Rankine-Hugoniot equations (5.3) should hold between any state in the uniform constant state ahead of the shock and any interior point of the reaction zone behind the shock. The Hugoniot curve now depends on the extent of the chemical reaction (reactant mass fraction $Y$), which varies continuously from 1 to 0, giving the generalization of (5.13)

$$p(v,Y) = \frac{2Q(1 - Y) - p_u v + \frac{\tau + 1}{\tau - 1} p_u v_u}{\frac{\tau + 1}{\tau - 1} v - v_u}. \quad (6.1)$$

The Hugoniot curves (6.1) for different values of $Y$ are drawn in Figure 4. The curve with $Y = 0$ corresponds to the states where the reaction is completed and all heat is released (see Figure 2).

![Figure 4: The Hugoniot curves corresponding to the ZND-theory.](image)

The single variable $Y$ completely defines the state as the state point moves down the Rayleigh line. Firstly, due to a non-reacting shock wave the pressure and density (and temperature) jump to a higher value on the Hugoniot curve $p(\cdot, 1)$, called the von Neumann spike (vN-spike) [7, 9]. The von Neumann spike is the state immediately behind the non-reacting shock wave and would be the final state if no chemical reaction takes place. As the reaction proceeds the state point moves down the Rayleigh line (pressure and density decrease) until the
reaction is completed and the final state on the Hugoniot curve \( p(\cdot, 0) \) is reached. At each point on the Rayleigh-line between the von Neumann spike and the final state there is a unique \( Y \) determined from the Rankine-Hugoniot equations. The corresponding values for the pressure \( p \) and specific volume \( v \) can be obtained from the Rankine-Hugoniot equations and the value of \( Y \). It can easily be verified that for a CJ or strong detonation

\[
\begin{align*}
p(Y) &= \frac{m^2 v_u + p_u}{\gamma + 1} + \frac{1}{\gamma + 1} \beta(Y), \quad (6.2a) \\
v(Y) &= \gamma \left( \frac{m^2 v_u + p_u}{\gamma + 1} - \frac{1}{m^2(\gamma + 1)} \beta(Y) \right), \quad (6.2b) \\
u(Y) &= s - v(Y)m,
\end{align*}
\]

where, for shortness of notation, \( \beta(Y) \) is introduced as

\[
\beta(Y) := \sqrt{(m^2 v_u - \gamma p_u)^2 - 2(\gamma^2 - 1)m^2 Q(1 - Y)}. \quad (6.2d)
\]

Note that \( p(0), v(0) \) and \( u(0) \) correspond to the final states given by (5.16) or (5.17).

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, \( g(\xi) = g_u \) for all \( \xi > 0 \) and all variables \( g \). Still the dependence of \( Y \) on the distance \( \xi \) has to be determined. Note that all variables can be expressed in terms of \( Y \), and, subsequently, also the reaction rate \( w \). Since we consider a steady flow (5.2) should hold. Using (5.2a) and (5.3a), equation (5.2d) implies that the mass fraction of the reactant \( Y \) is given by the following ordinary differential equation

\[
\begin{align*}
\frac{d}{d\xi} Y(\xi) &= -\frac{w(Y(\xi))}{m}, \quad \forall \xi < 0, \quad (6.3a) \\
Y(0) &= 1, \quad (6.3b)
\end{align*}
\]

where \( \xi = 0 \) corresponds to the position of the precursor shock. In general, (6.3) can not be solved exactly and the solution must be obtained numerically. If we have computed \( Y \), then we can determine all other variables from (6.2).

Note that for the ZND-model the final state is a strong or CJ detonation. There is no path from the von Neumann spike to a point on the Hugoniot curve with \( Y = 0 \), corresponding to a weak detonation. It is obvious from Figure 4 that there can also be a shockless steady state solution with \( Y \) decreasing up to the Rayleigh line from the initial point \((v_u, p_u)\) to a weak detonation point. In the present context the reaction rate would have to be finite in the initial state, without a shock to start it (contrary to assumption A15). Therefore, we restrict ourselves to strong or CJ detonations [5, 9].

The minimum speed for a detonation is the speed \( s_{CL} \) of a CJ detonation [5, 7, 9]. 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 [2]

\[
f := \left( \frac{s}{s_{CL}} \right)^2, \quad (6.4)
\]

from which it directly follows that \( f \geq 1 \). Suppose that all states ahead of the detonation wave are known. Furthermore the parameters \( Da, E_\alpha, f, Q \) and \( \gamma \) are known. Firstly, we compute \( m_{CL} \) using (5.15). Subsequently, \( m_{CL} \) and (5.3a) give the speed \( s_{CL} \) of a CJ detonation.
Using the degree of overdrive $f$ we can compute the detonation speed as $s = s_{CJ} \sqrt{f}$. After computing $m$ by (5.3a) and solving (6.3) the complete ZND-solution is derived (see (6.2)).

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 [7]. Often the Damköhler number $Da$ in the reaction rate (4.5) is used to normalise the rate equation such that $L_{1/2} = 1$ [2, 7]. It is easy to see that (6.3) implies that $L_{1/2}$ is given by

$$L_{1/2} = -m \int_{1/2}^{1} \frac{1}{w(Y)} dY.$$ \hspace{1cm} (6.5)

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

![Figure 5: ZND-solution of (4.2), with $E_a = 14, f = 1, Q = 14, \gamma = 1.4$ and $Da = 0.6488$.](image)

**Example 6.1** As an example of the preceding theory we describe the ZND-solution of the CJ detonation discussed in [1]. All quantities are nondimensionalised with respect to the unburnt gas. Hence, the dimensionless preshock state is given by

$$p_u = 1, \quad p_{\infty} = 1, \quad u_u = 0.$$  

Furthermore, we have the following parameter values

$$E_a = 14, \quad Q = 14, \quad f = 1, \quad \gamma = 1.4.$$
Finally, the Damköhler number $Da$ is chosen such that $L_{1/2} = 1$. It follows from (5.3a), (5.15) and (5.16) that the final state for the CJ detonation is given by

$$p_b = p_{CJ} = 12.756, \quad \rho_b = \rho_{CJ} = 1.6583, \quad u_b = u_{CJ} = 2.1602,$$

where the CJ detonation is propagating with a speed $s = s_{CJ} = 5.4419$. In Figure 5 the steady ZND-solution is drawn. The pressure reaches its maximum value right behind the precursor shock. As mentioned before this value is called the von Neumann spike, which in this particular case satisfies $p_{vN} = p(0) = 24.512$ (see (6.2a)).

The maximum of the temperature near the end of the reaction zone can be explained by the geometry of the isotherms near the CJ point (see Figure 6). The Rayleigh line is tangent to the Hugoniot curve at the CJ point. The isotherms are less steep but concave upward, so precisely one of them will be tangent to the Rayleigh line somewhere above the CJ point [6, 7]. If this point of tangency lies below the von Neumann spike, the steady state solution will have a maximum in the temperature. Finally, Figure 5 clearly shows that the reaction rate $w$ is zero ahead of the shock and finite behind it (as assumed in A15).

![Figure 6: Explanation of temperature maximum in the ZND-solution.](image)

**Example 6.2** As a second example the ZND-solution of a strong detonation is described [1, 2, 7]. Again, all quantities are nondimensionalised with respect to the unburnt gas. Hence, the dimensionless preshock state is given by

$$p_u = 1, \quad \rho_u = 1, \quad u_u = 0.$$

The dimensionless parameters are

$$E_a = 50, \quad Q = 50,$$

$$f = 1.8, \quad \gamma = 1.2.$$
Finally, the Damköhler number $Da$ is chosen such that $L_{1/2} = 1$. It follows from (5.3a), (5.15) and (5.17) that the final state for the strong detonation is given by

$$p_b = p_{CJ} = 63.680, \quad \rho_b = \rho_{CJ} = 4.0158,$$

$$u_b = u_{CJ} = 6.8609,$$

where the strong detonation is propagating with a speed $s = s_s = 9.1359$. In Figure 7 the steady ZND-solution is drawn. In this particular case the von Neumann spike satisfies $p_{vN} = p(0) = 75.786$ (see (6.2a)).

![Figure 7: ZND-solution of (4.2), with $E_a = 50$, $f = 1.8$, $Q = 50$, $\gamma = 1.2$ and $Da = 0.2557$.](image-url)
### Appendix: Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>frequency factor ($s^{-1}$)</td>
</tr>
<tr>
<td>$B$</td>
<td>constant in frequency factor ($s^{-1}K^{-\alpha}$)</td>
</tr>
<tr>
<td>$c$</td>
<td>speed of sound (m/s)</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure of the gas mixture ($J/(kg\ K)$)</td>
</tr>
<tr>
<td>$c_{p,i}$</td>
<td>specific heat at constant pressure for species $M_i$ ($J/(kg\ K)$)</td>
</tr>
<tr>
<td>$c_v$</td>
<td>specific heat at constant volume of the gas mixture ($J/(Kg\ K)$)</td>
</tr>
<tr>
<td>$D$</td>
<td>constant binary diffusion coefficient for all pairs of species ($m^2/s$)</td>
</tr>
<tr>
<td>$D_{ij}$</td>
<td>binary diffusion coefficient for species $M_i$ and $M_j$ ($m^2/s$)</td>
</tr>
<tr>
<td>$D_a$</td>
<td>Damköhler number</td>
</tr>
<tr>
<td>$e$</td>
<td>specific internal energy per unit mass for the gas mixture ($J/kg$)</td>
</tr>
<tr>
<td>$E$</td>
<td>specific total energy per unit mass for the gas mixture ($J/kg$)</td>
</tr>
<tr>
<td>$E_a$</td>
<td>activation energy ($J/mol$)</td>
</tr>
<tr>
<td>$f$</td>
<td>degree of overdrive</td>
</tr>
<tr>
<td>$f_i$</td>
<td>external force per unit mass on species $M_i$ ($N/kg$)</td>
</tr>
<tr>
<td>$h$</td>
<td>specific enthalpy of the gas mixture ($J/kg$)</td>
</tr>
<tr>
<td>$h_i$</td>
<td>specific enthalpy of species $M_i$ ($J/kg$)</td>
</tr>
<tr>
<td>$h_i^0$</td>
<td>standard heat of formation per unit mass for species $M_i$ at temperature $T_0$ ($J/kg$)</td>
</tr>
<tr>
<td>$k$</td>
<td>specific rate constant ($s^{-1}$)</td>
</tr>
<tr>
<td>$L_{1/2}$</td>
<td>half reaction length (m)</td>
</tr>
<tr>
<td>$m$</td>
<td>mass flux ($kg/(m^2\ s)$)</td>
</tr>
<tr>
<td>$p$</td>
<td>hydrostatic pressure ($N/m^2$)</td>
</tr>
<tr>
<td>$q$</td>
<td>heat flux for the gas mixture ($J/(m^2\ s)$)</td>
</tr>
<tr>
<td>$Q$</td>
<td>heat release of the chemical reaction per unit mass ($J/kg$)</td>
</tr>
<tr>
<td>$R$</td>
<td>universal gas constant ($J/(mol\ K)$)</td>
</tr>
<tr>
<td>$S$</td>
<td>specific entropy of the gas mixture ($J/(Kg\ K)$)</td>
</tr>
<tr>
<td>$T$</td>
<td>absolute temperature of the gas mixture (K)</td>
</tr>
<tr>
<td>$T_0$</td>
<td>fixed reference temperature (K)</td>
</tr>
<tr>
<td>$u$</td>
<td>mass weighted average velocity of the gas mixture (m/s)</td>
</tr>
<tr>
<td>$u_i$</td>
<td>flow velocity of species $M_i$ (m/s)</td>
</tr>
<tr>
<td>$U_i$</td>
<td>diffusion velocity of species $M_i$ (m/s)</td>
</tr>
<tr>
<td>$v$</td>
<td>specific volume of the gas mixture ($m^3/kg$)</td>
</tr>
<tr>
<td>$w_i$</td>
<td>reaction rate of species $M_i$ ($kg/(m^3\ s)$)</td>
</tr>
<tr>
<td>$W$</td>
<td>average molecular weight of the gas mixture ($kg/mol$)</td>
</tr>
<tr>
<td>$W_i$</td>
<td>molecular weight of species $M_i$ ($kg/mol$)</td>
</tr>
<tr>
<td>$X_i$</td>
<td>mole fraction of species $M_i$</td>
</tr>
<tr>
<td>$Y_i$</td>
<td>mass fraction of species $M_i$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>constant determining the temperature dependence of the frequency factor</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>thermal conductivity of the gas mixture ($J/(m\ s\ K)$)</td>
</tr>
<tr>
<td>$\mu$</td>
<td>viscosity coefficient ($kg/(m\ s)$)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>specific heat ratio</td>
</tr>
<tr>
<td>$\rho$</td>
<td>mass density of the gas mixture ($kg/m^3$)</td>
</tr>
<tr>
<td>$\rho_i$</td>
<td>mass density of species $M_i$ ($kg/m^3$)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>stress of the gas mixture ($N/m^2$)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>viscous stress of the gas mixture ($N/m^2$)</td>
</tr>
</tbody>
</table>
References


