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INTRODUCTION TO COMBUSTION MODELLING

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INTRODUCTION TO COMBUSTION MODELLING

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The following Notes summarize the lectures given by the author at the Workshop on Theoretical Fluid Mechanics held at the International Centre for Theoretical Physics in Trieste, in January 1989.

These Notes consist of the first chapter and of the reference list of the monograph "Introduction to mathematical and numerical modelling in gaseous combustion", which will be published by Gordon & Breach (in the series "Applied Mathematics") in early 1989. This first chapter reviews the most classical models used in combustion theory. For more details on the subjects presented during the lectures, the participants are referred to the above mentioned monograph or to the reference list; references followed by "N" (resp. "M") more precisely concern numerical studies (resp. mathematical studies).

CHAPTER ONE

THE MATHEMATICAL MODELS

We present in this chapter the systems of partial or ordinary differential equations whose mathematical and numerical investigation is the subject of this book. We first briefly recall how the basic governing equations of gaseous reactive flows are derived from fundamental physical theories, and we present the main approximations of these systems which are classically used to describe premixed flame propagation. We conclude this introductive chapter by giving a short description of the structure of a premixed flame, in the steady one-dimensional case.

1. THE BASIC EQUATIONS OF GASEOUS REACTIVE FLOW

The problem is therefore to describe the flow of a *compressible gaseous mixture* made of several *chemically reactive* species, while taking into account the effects of *species diffusion* and *heat conduction*.

The most rigorous way of obtaining a model including all these effects is to derive it in the framework of the kinetic gas theory, starting with the Liouville or Boltzmann equations (see Hirschfelder et al [71], Williams [149]). Nevertheless, the same system of governing equations can be derived in the simpler framework of continuum mechanics, at the price of some simplifying hypotheses. We now briefly describe this second approach.

1.1. The general approach

We therefore consider the flow of a mixture of N gaseous species $\mathcal{A}_k$, $1 \leq k \leq N$ (the subscript k will always denote a species). The derivation of the governing equations of this flow relies on the following hypothesis: we assume that N "continuous media"

(or "continua") coexist in the mixture, corresponding to the N different species. We therefore have, at each point $\vec{x}$ and at each time t, N separate densities $\rho_k(\vec{x},t)$, N velocities $\vec{v_k}(\vec{x},t)$, N partial pressures $p_k(\vec{x},t)$; we assume that these variables are continuous and even continuously differentiable with respect to the space and time coordinates. We also define the mixture density ρ by the relation $\rho(\vec{x},t) = \sum_k \rho_k(\vec{x},t)$, the "mixture velocity" $\vec{v}$ by $\rho\vec{v} = \sum_k \rho_k\vec{v_k}$, and the total pressure p by $p = \sum_k p_k$ (Dalton's law). Lastly, we assume the local thermal equilibrium between all species at each point, or in other words that the temperature is the same for all species $T_k(\vec{x},t) = T(\vec{x},t)$.

The approach now consists in writing the equations of fluid mechanics for each of the species, and in deriving equations for the mixture in a second step. For instance, the conservation of mass for the k^{th} continuum takes the form:

$$(\rho_k)_t + \vec{\nabla}.(\rho_k\vec{v_k}) = \dot{\rho}_k \ , \tag{1.1}$$

where $\dot{\rho}_k$ is the rate of variation of the separate density of species $\mathcal{A}_k$ due to chemical reactions (consumption or production rate, as the case may be). Summing these equations for all species, and using the relation $\sum_{k=1}^{N} \dot{\rho}_k = 0$ which expresses that the chemical reactions do not create mass, we obtain for the mixture the usual form of the continuity equation:

$$\rho_t + \vec{\nabla}.(\rho\vec{v}) = 0 \ . \tag{1.2}$$

The momentum and energy equations can be treated in the same way to give the following system:

$$\begin{cases} \rho_t + \vec{\nabla}.(\rho\vec{v}) = 0 \ , \\ (\rho v_i)_t + \vec{\nabla}.(\rho v_i\vec{v}) = \rho F_i + \sigma_{ij,j} \ , \\ (\rho\epsilon + \frac{1}{2}\rho U^2)_t + \vec{\nabla}.[(\rho\epsilon + \frac{1}{2}U^2)\vec{v}] = (\sigma_{ij}v_i)_j + \rho F_i v_i - \vec{\nabla}.\vec{q} \ , \\ (\rho_k)_t + \vec{\nabla}.(\rho_k\vec{v}) = \dot{\rho}_k - \vec{\nabla}.(\rho_k\vec{V_k}) \ . \end{cases} \tag{1.3}$$

We have used classical notations: $\vec{F}$ denotes the external body forces per unit mass, σ_{ij} are the components of the mixture stress tensor, ϵ is the internal energy per unit mass of the mixture ($\rho\epsilon = \sum_k \rho_k\epsilon_k$), and $U = \sqrt{\vec{v}.\vec{v}}$ is the fluid velocity. Furthermore, $\vec{q}$ denotes the energy flux, and $\vec{V_k} = \vec{v_k} - \vec{v}$ is the *diffusion velocity* of the species

$\mathcal{A}_k$. As usual, the time subscript t and the space subscripts i and j denote a partial derivative when appearing after a comma or a parenthesis.

In the case of a three-dimensional reactive flow, (1.3) is a system of $N+5$ equations; it is therefore convenient to consider as independent variables the $N+5$ quantities ρ, v_i $(1 \le i \le 3)$, T, and the mass fractions Y_k $(1 \le k \le N)$ of the species, defined by the identities $\rho_k = \rho Y_k$. To close the model, we still have to give, or to express in terms of the independent variables, the remaining terms: $\vec{F}$, σ_{ij}, ϵ, $\vec{q}$, $\dot{\rho}_k$ and $\vec{V_k}$.

The first three terms in this list are treated in a very classical way. The external forces are usually given (for example $\vec{F} = \vec{g}$ for gravity effects). Moreover, we assume for simplicity that each species behaves as a perfect gas and that the mixture is Newtonian, by writing:

$$\sigma_{ij} = -(p + \frac{2}{3}\mu\vec{\nabla}.\vec{v})\delta_{ij} + \mu(v_{i,j} + v_{j,i}) \ , \tag{1.4}$$

where μ is the mixture viscosity, the pressure p being given by Dalton's law:

$$p = \sum_k p_k = \rho RT\sum_k \frac{Y_k}{m_k} \ , \tag{1.5}$$

R and m_k denoting respectively the universal gas constant and the molecular weight of species $\mathcal{A}_k$. Lastly, we have the following classical thermodynamic relations:

$$\begin{aligned} \epsilon &= \sum_k Y_k\epsilon_k = \sum_k Y_k(h_k - \frac{p_k}{\rho_k}) \ , \\ &= \sum_k Y_k h_k^0 + \sum_k Y_k \int_{T_0}^{T} C_p^k dT - \frac{p}{\rho} \ , \end{aligned} \tag{1.6}$$

where h_k is the specific enthalpy of the species $\mathcal{A}_k$ at temperature T, h_k^0 its specific heat of formation at the reference temperature T_0, and C_p^k its specific heat at constant pressure.

1.2. Diffusion and reaction effects

At this stage, it remains to evaluate the energy and species diffusion terms ($\vec{q}$ and $\rho_k\vec{V_k}$), as well as the chemical reaction terms ($\dot{\rho}_k$), which rarely or never appear in the models of classical (non reactive) gas dynamics.

For the transport effects, we will use the following simplest laws:

$$\overrightarrow{q} = -\lambda \overrightarrow{\nabla T} + \sum_k \rho_k h_k \overrightarrow{V_k} , \tag{1.7}$$

which expresses the energy flux $\overrightarrow{q}$ as the sum of a conductive heat flux (λ is the mixture thermal conductivity) and of the diffusive enthalpy fluxes of all species, and:

$$\rho_k \overrightarrow{V_k} = -\rho D \overrightarrow{\nabla Y_k} , \tag{1.8}$$

where $D > 0$ is a diffusion coefficient. These relations, which follow from Fourier's and Fick's law, can be seen either as empirical, or as simplified expressions of the much more complex models obtained in the framework of kinetic gas theory (see Williams [149]).

Let us finally express the reaction terms $\dot{\rho}_k$, in the case where a single chemical reaction, written as:

$$\sum_k \mu_k \mathcal{A}_k \longrightarrow \sum_k \nu_k \mathcal{A}_k \tag{1.9}$$

takes place in the mixture. The natural integers μ_k and ν_k are the stoechiometric coefficients of the reaction (a typical example of reaction of type (1.9) is the global reaction for the combustion of hydrogen: $2\ H_2 + O_2 \longrightarrow 2\ H_2O$).

It follows from (1.9) that the rates of variation $\dot{\rho}_k$ of the separate densities of the different species are related to each other by an identity of the form:

$$\forall\ k,\ \frac{\dot{\rho}_k}{m_k(\nu_k - \mu_k)} = \omega\ ; \tag{1.10}$$

ω is the global reaction rate of reaction (1.9) (and is independent of k).

The theoretical evaluation of this global rate ω is a difficult problem, which involves quantum physics and is still the subject of numerous fundamental investigations. To make the problem more precise, consider the simple case of a reaction $\mathcal{A} + \mathcal{B} \longrightarrow Products$. At the molecular level, the reaction only proceeds during a collision of a molecule $\mathcal{A}$ and a molecule $\mathcal{B}$, *provided that* this collision is sufficiently energetic (i.e. such that the "kinetic energy of the relative motion" of the two colliding molecules is large enough), and *provided that* the "relative orientation" of the colliding molecules allows the reaction to proceed (see e.g. [93], Sivashinsky [127], Vincenti-Kruger [144]). Now, the kinetic gas theory allows one to evaluate the number

of collisions of molecules $\mathcal{A}$ and $\mathcal{B}$ per units time and volume (the so called "collision rate", obtained from Maxwell's distribution of the molecules velocities), and even the number of those collisions which are sufficiently energetic. But of course, this theory, in which the molecules are seen as solid spheres, cannot consider the second condition: the "steric factor", i.e. the fraction of the sufficiently energetic collisions which actually produce the chemical reaction, can only be evaluated using Schrödinger's equation, or measured experimentally.

Nevertheless, one may think that the expression of the collision rate gives the main terms appearing in the chemical reaction rate ω. For the reaction (1.9), one obtains:

$$\omega = \prod_k \left(\frac{\rho Y_k}{m_k}\right)^{\mu_k} F(T) . \tag{1.11}$$

The way in which the mass fractions Y_k appear in this expression is referred to as the law of mass action. The function $F(T)$ has the form:

$$F(T) = B(T) \exp\left(-\frac{\mathcal{E}}{RT}\right) , \tag{1.12}$$

where $B(T)$ is an algebraic function of T, and where the positive constant $\mathcal{E}$ is the activation energy of the reaction; the exponential term in (1.12) is called the Arrhenius term.

1.3. Governing equations of reactive flows

We have now given the expression of all terms appearing in system (1.3).

Usually, the description of a gaseous reactive flow requires to take into account a very large number (one or several tens) of species and of chemical reactions (see e.g. Clavin [40], Giovangigli [66], Warnatz [146]): the system (1.3) then includes a large number of equations and of nonlinear reaction source terms expressing the consumption or production of the species by the different chemical reactions.

Throughout this book, we will avoid the difficulties related to complex chemical mechanisms by assuming that the mixture is made up of only two species $\mathcal{R}$ and $\mathcal{P}$, whose mass fractions will be denoted $Y_{\mathcal{R}} = Y$ and $Y_{\mathcal{P}} = 1 - Y$ respectively, and that a single one-step exothermic chemical reaction of the form:

$$\mathcal{R} \longrightarrow \mathcal{P} \tag{1.13}$$

takes place in the gas. Using the relations (1.4)-(1.12), and neglecting for simplicity the viscous terms and the external forces, we can rewrite the system (1.3) as:

$$\begin{cases} \rho_t + \vec{\nabla}.(\rho\vec{v}) = 0\ , \\ (\rho v_i)_t + \vec{\nabla}.(\rho v_i\vec{v}) = -p_{,i}\ , \\ E_t + \vec{\nabla}.[(E+p)\vec{v}] = \vec{\nabla}.(\lambda\vec{\nabla T}) + Q\vec{\nabla}.(\rho D\vec{\nabla Y})\ , \\ (\rho Y)_t + \vec{\nabla}.(\rho Y\vec{v}) = -m\omega(\rho Y,T) + \vec{\nabla}.(\rho D\vec{\nabla Y})\ , \\ mp = \rho RT\ ,\ \ \omega(\rho Y,T) = \dfrac{\rho Y}{m}F(T)\ ; \end{cases} \tag{1.14}$$

the constant $Q = h^0_{\mathcal{R}} - h^0_{\mathcal{P}} > 0$ is the heat released by the reaction (1.13) per unit mass of reactant, and

$$E = \rho\epsilon + \frac{1}{2}\rho U^2 = Q\rho Y + \rho C_v T + \rho(h^0_{\mathcal{P}} - C_p T_0) + \frac{1}{2}\rho U^2 \tag{1.15}$$

is the total energy per unit volume. We have used the fact that both species $\mathcal{R}$ and $\mathcal{P}$ have the same molecular weight m and the same constant specific heats C_p and C_v (which satisfy Mayer's relation $m(C_p - C_v) = R$).

This system can be rewritten under several equivalent forms. The following conservative formulation:

$$\begin{cases} \rho_t + \vec{\nabla}.(\rho\vec{v}) = 0\ , \\ (\rho v_i)_t + \vec{\nabla}.(\rho v_i\vec{v}) = -p_{,i}\ , \\ e_t + \vec{\nabla}.[(e+p)\vec{v}] = \vec{\nabla}.(\lambda\vec{\nabla T}) + mQ\omega(\rho Y,T)\ , \\ (\rho Y)_t + \vec{\nabla}.(\rho Y\vec{v}) = -m\omega(\rho Y,T) + \vec{\nabla}.(\rho D\vec{\nabla Y})\ , \\ mp = \rho RT\ ,\ \ \omega(\rho Y,T) = \dfrac{\rho Y}{m}F(T)\ , \end{cases} \tag{1.16}$$

where:

$$e = \rho C_v T + \frac{1}{2}\rho U^2\ , \tag{1.17}$$

is the sum of the thermal and kinetic energies, will be used for numerical studies in Chapter 6. The next equivalent system, written in non conservative form, is more classically used by the physicists interested in flame propagation, and will be shown in the next section to lead to the simplified models investigated in Chapters 2 to 5:

$$\begin{cases} \rho_t + \vec{\nabla}.(\rho\vec{v}) = 0\ , \\ \rho v_{i,t} + \rho\vec{v}.\vec{\nabla v_i} = -p_{,i}\ , \\ \rho C_p T_t + \rho C_p\vec{v}.\vec{\nabla T} = mQ\omega(\rho Y,T) + \vec{\nabla}.(\lambda\vec{\nabla T}) + p_t + \vec{v}.\vec{\nabla p}\ , \\ \rho Y_t + \rho\vec{v}.\vec{\nabla Y} = -m\omega(\rho Y,T) + \vec{\nabla}.(\rho D\vec{\nabla Y})\ , \\ mp = \rho RT\ ,\ \ \omega(\rho Y,T) = \dfrac{\rho Y}{m}F(T)\ . \end{cases} \tag{1.18}$$

Notice that in systems (1.16) and (1.18), the non linear reaction term $\omega(\rho Y,T)$ now appears in the energy equation as well as in the mass fraction equation.

Thus, the systems (1.14), (1.16) and (1.18) describe the gaseous reactive flow of two species, under the above mentioned hypotheses (one-step chemistry, no external forces or viscous effects...). Even with these simplifying assumptions, these systems describe phenomena which are very different from each other, such as deflagrations and detonations (see Courant-Friedrichs [44]); they involve many physical effects (reaction, diffusion, conduction, gas expansion and acoustics...), most of them being non linear and strongly coupled.

These models are used in several numerical studies (see Chapter 6 and the references therein), but their rigorous mathematical analysis is presently out of reach. This is the reason why we introduce in the next section some *simplified* models, which are classically used in combustion theory (and also for numerical experiments). All these simplified models will be shown to lead to some decoupling between the reactive and diffusive effects on one hand and the hydrodynamical effects on the other hand; their mathematical analysis will be presented in Chapters 2 and 3, while their numerical solution is the object of Chapters 4 and 5.

2. CLASSICAL APPROXIMATIONS OF COMBUSTION THEORY

2.1. The isobaric approximation

2.1.1. The isobaric model

The most classical approximation used to study slow combustion (i.e. deflagrations, or flames) relies on the highly subsonic character of these phenomena: the value

of a representative Mach number Ma is of the order of 10^{-2}. A *formal* expansion of the variables in powers of the small parameter Ma then shows that the pressure is constant in space up to second order, which means that:

$$p(\vec{x},t) = P(t) + \tilde{p}(\vec{x},t) \ , \tag{1.19}$$

with $\frac{\tilde{p}}{P} = O(Ma^2) \ll 1$ (see for instance Buckmaster-Ludford [36], Ghilani [62], Joulin [77]). The same formal expansion also shows that the pressure gradient $\vec{\nabla}p$ is negligible with respect to the other terms in the energy balance equation (1.18.c), but not in the momentum equation (1.18.b). If the combustion takes place inside an open vessel, the pressure $P(t)$ is constant: $P(t) = P_0$ (for instance the atmospheric pressure); on the opposite, P actually depends on time if the burning mixture is confined inside a closed chamber.

From now on, we will assume that the combustion of the mixture of both species $\mathcal{R}$ and $\mathcal{P}$ appearing in (1.13) occurs inside a two-dimensional infinite rectangular open tube S of width L, $S = \{(x,y) \in \mathbb{R}^2, \ 0 < y < L\}$. Denoting now u and v the components of the mixture velocity $\vec{v}$ and using the above considerations (i.e. neglecting the spatial pressure variations), we describe the propagation of a flame in the tube S by the *isobaric model*:

$$\begin{cases} \rho_t + (\rho u)_x + (\rho v)_y = 0 \ . \\ \rho u_t + \rho u u_x + \rho v u_y = -p_x \ , \\ \rho v_t + \rho u v_x + \rho v v_y = -p_y \ , \\ \rho C_p T_t + \rho C_p u T_x + \rho C_p v T_y = mQ\omega(\rho Y, T) + \vec{\nabla}.(\lambda \vec{\nabla} T) \ , \\ \rho Y_t + \rho u Y_x + \rho v Y_y = -m\omega(\rho Y, T) + \vec{\nabla}.(\rho D \vec{\nabla} Y) \ , \\ \rho RT = mP_0 \ , \ \ \omega(\rho Y, T) = \dfrac{\rho Y}{m} F(T) \ . \bullet \end{cases} \tag{1.20}$$

Remark 1.1: Another model is also proposed by Majda [98] to describe the combustion of a gaseous mixture confined in a closed vessel in the limit of zero Mach number. The mathematical analysis of this system, in which the reactive, diffusive and hydrodynamical effects remain coupled, has been carried out by Embid [53], using techniques similar to those employed for investigating the Navier-Stokes equations (see e.g. Temam [140]). •

2.1.2. The one-dimensional steady case

We have not mentioned for the moment the boundary conditions associated to the isobaric model (1.20). We now derive these conditions by considering one-dimensional steady solutions of this model, which will be shown to be simply given by a system of two ordinary differential equations.

Indeed, the mass conservation equation (1.20.a) writes in the one-dimensional steady case:

$$(\rho u)_x = 0 \ , \tag{1.21}$$

whence $\rho u = c$, an unknown constant. Setting $G(T) = \frac{mP_0}{RT} F(T)$, we can then rewrite (1.20) under the form:

$$\begin{cases} cC_p T_x = QYG(T) + (\lambda T_x)_x \ , \\ cY_x = -YG(T) + (\rho D Y_x)_x \ , \end{cases} \tag{1.22}$$

$$\begin{cases} \rho = \dfrac{mP_0}{RT} \ , \\ u = \dfrac{c}{\rho} \ , \\ p_x = -cu_x \ . \end{cases} \tag{1.23}$$

The equations (1.22) are therefore decoupled from (1.23): as will be seen in the next chapter, equations (1.22) (together with the associated boundary conditions) determine T, Y *and the constant* c, the variables ρ, u and p being given in a second step by (1.23).

When one considers the *propagation of a flame* inside the tube S (that is, the particular form of combustion which takes place when the ignition of the mixture occurs at one point inside the tube or in some part of it), the boundary conditions associated to equations (1.22) are of the following type:

$$\begin{cases} T(-\infty) = T_u \quad (0 < T_u) \ , \\ Y(-\infty) = Y_u \quad (0 < Y_u < 1) \ , \\ T(+\infty) = T_b \quad (T_u < T_b) \ , \\ Y(+\infty) = 0 \ ; \end{cases} \tag{1.24}$$

T_u and Y_u respectively denote the temperature and the mass fraction of reactant in the fresh mixture in which the flame propagates, and T_b is the burnt gas temperature; the last condition expresses that the combustion is complete: there remains no reactant behind the flame (see the Figure 1.1 below for a representation of the solutions of

(1.22)). Furthermore, the burnt gas temperature is simply given by writing the overall energy balance equation (obtained by integrating from $-\infty$ to $+\infty$ the sum of the first equation (1.22.a) and of the second equation (1.22.b) multiplied by Q):

$$T_b = T_u + \frac{QY_u}{C_p} . \tag{1.25}$$

This relation can be used to rewrite system (1.22) under a very simple normalized form; assuming that the positive quantities λ and $Le = \frac{\lambda}{\rho C_p D}$ (Lewis number) are constant, and introducing the normalized variables $\Theta = \frac{T - T_u}{T_b - T_u}$, $Z = \frac{Y}{Y_u}$ and $x' = \frac{C_p}{\lambda} x$, we obtain for (1.22) and (1.24) the following equations:

$$\begin{cases} c\Theta_{x'} = Z f(\Theta) + \Theta_{x'x'} , \\ cZ_{x'} = -Z f(\Theta) + \frac{1}{Le} Z_{x'x'} \quad \text{on } \mathbb{R} , \end{cases} \tag{1.26}$$

$$\begin{cases} \Theta(-\infty) = 0 , \quad Z(-\infty) = 1 , \\ \Theta(+\infty) = 1 , \quad Z(+\infty) = 0 , \end{cases} \tag{1.27}$$

where $f(\Theta) = \frac{\lambda}{C_p} G(T)$. The mathematical analysis of this model (1.26)-(1.27) is briefly presented in the next chapter.

2.1.3. The one-dimensional unsteady case

We now consider the one-dimensional *unsteady* solutions of the isobaric model (1.20); these solutions are given by the following system, written here under conservative form:

$$\begin{cases} \rho_t + (\rho u)_x = 0 , \\ (\rho u)_t + (\rho u^2)_x = -p_x , \\ (\rho C_p T)_t + (\rho u C_p T)_x - (\lambda T_x)_x = mQ\omega(\rho Y, T) , \\ (\rho Y)_t + (\rho u Y)_x - (\rho D Y_x)_x = -m\omega(\rho Y, T) . \\ \\ \rho RT = mP_0 , \quad \omega(\rho Y, T) = \frac{\rho Y}{m} F(T) . \end{cases} \tag{1.28}$$

It will be shown in Chapter 2 that this system of nonlinear partial differential equations forms a well-posed mathematical problem when associated to boundary conditions similar to (1.24):

$$\begin{cases} T(-\infty, t) = T_u , \quad Y(-\infty, t) = Y_u , \\ T(+\infty, t) = T_b , \quad Y(+\infty, t) = 0 , \end{cases} \tag{1.29}$$

and to the following additional initial and boundary conditions:

$$T(x,0) = T_0(x) , \quad Y(x,0) = Y_0(x) , \tag{1.30}$$

$$u(-\infty, t) = u_u , \quad p(-\infty, t) = p_u , \tag{1.31}$$

where u_u and p_u are given constants (the reasons for choosing these initial and boundary conditions will clearly appear in Chapter 2).

In fact, the investigation of the solutions of (1.28)-(1.31), both from a mathematical and a numerical point of view, uses instead of (1.28) the Lagrangian form of (1.28), which we now derive using the usual mass-weighted Lagrangian coordinate:

$$\xi = \int_{x(0,t)}^{x(\xi,t)} \rho(x', t)\, dx' \tag{1.32}$$

(see Courant-Friedrichs [44]). Although the use of this transformation is classical, we detail the calculation for sake of completeness. We first define a Lagrangian coordinate (i.e. a variable whose value, defined at time $t = 0$, remains constant during the flow for each fluid particle) by setting:

$$\xi = \int_0^x \rho(x', 0) dx' . \tag{1.33}$$

We also set $\tau = t$. Then $\xi(x,t)$ represents the Lagrangian coordinate of the particle which is located at the abcissa x at time t and the last relation is to be read as $\xi(x,0) = \int_0^x \rho(x',0)dx'$. Inversely, $x(\xi, \tau)$ is the position at time τ of the fluid particle whose Lagrangian coordinate is ξ. Therefore we have, by definition:

$$x_\tau = u , \quad \text{or } \frac{\partial}{\partial \tau} x(\xi, \tau) = u[x(\xi, \tau), \tau] . \tag{1.34}$$

We can then write:

$$\begin{aligned} \frac{d}{d\tau}\left[\int_{x(0,\tau)}^{x(\xi,\tau)} \rho(x',\tau)dx'\right] &= \frac{\partial x}{\partial \tau}(\xi,\tau)\rho[x(\xi,\tau),\tau] - \frac{\partial x}{\partial \tau}(0,\tau)\rho[x(0,\tau),\tau] \\ &\quad + \int_{x(0,\tau)}^{x(\xi,\tau)} \frac{\partial \rho}{\partial \tau}(x',\tau)dx' , \\ &= (\rho u)[x(\xi,\tau),\tau] - (\rho u)[x(0,\tau),\tau] + \int_{x(0,\tau)}^{x(\xi,\tau)} \frac{\partial \rho}{\partial \tau}(x',\tau)dx' , \\ &= \int_{x(0,\tau)}^{x(\xi,\tau)} [\rho_\tau + (\rho u)_{x'}](x',t)dx' = 0 , \end{aligned} \tag{1.35}$$

from (1.28.a), whence:

$$\int_{x(0,\tau)}^{x(\xi,\tau)} \rho(x',\tau)dx' = \int_{x(0,0)}^{x(\xi,0)} \rho(x',0)dx' = \xi \ , \tag{1.36}$$

which is exactly (1.32).

Differentiating (1.32) with respect to ξ gives:

$$1 = \rho x_\xi \ , \quad \text{or} \quad \frac{\partial}{\partial \xi} x(\xi,\tau) = \frac{1}{\rho[x(\xi,\tau),\tau]} \ . \tag{1.37}$$

We then have in matrix form (writing simply $u(\xi,\tau)$ for $u[x(\xi,\tau),\tau]$):

$$\begin{pmatrix} x_\xi & x_\tau \\ t_\xi & t_\tau \end{pmatrix} = \begin{pmatrix} \rho^{-1} & u \\ 0 & 1 \end{pmatrix} \ , \tag{1.38}$$

which implies:

$$\begin{pmatrix} \xi_x & \xi_t \\ \tau_x & \tau_t \end{pmatrix} = \begin{pmatrix} \rho & -\rho u \\ 0 & 1 \end{pmatrix} \ . \tag{1.39}$$

Remark 1.2: The mass balance equation (1.28.a) has been crucial for introducing the new variable ξ. This amounts to noticing that a variable ζ satisfying $\zeta_x = \rho$, $\zeta_t = -\rho u$ [i.e. (1.39)] could have been introduced directly, since (1.28.a) insures that $\frac{\partial}{\partial t}(\zeta_x) = \frac{\partial}{\partial x}(\zeta_t)$. •

We can now derive the Lagrangian form of the flame propagation equations (1.28). For any quantity F we have $F_t = F_\tau - \rho u F_\xi$, $F_x = \rho F_\xi$, and (1.28) becomes:

$$\begin{cases} \rho_\tau + \rho^2 u_\xi = 0 \ , \\ u_\tau + p_\xi = 0 \ , \\ T_\tau = \dfrac{mQ}{C_p}\dfrac{\omega(\rho Y,T)}{\rho} + \dfrac{1}{C_p}(\lambda \rho T_\xi)_\xi \ , \\ Y_\tau = -m\dfrac{\omega(\rho Y,T)}{\rho} + (\rho^2 D Y_\xi)_\xi \ , \\ \rho RT = mP_0 \ , \ \ \omega(\rho Y,T) = \dfrac{\rho Y}{m} F(T) \ . \end{cases} \tag{1.40}$$

Assuming as above that the Lewis number $Le = \dfrac{\lambda}{\rho C_p D}$ is constant, and assuming also that the ratio $\dfrac{\lambda}{T}$ is constant, we can rewrite (1.40) as:

$$\begin{cases} T_\tau = \dfrac{Q}{C_p} Y F(T) + \dfrac{mP_0}{RC_p}\dfrac{\lambda}{T}(T_\xi)_\xi \ , \\ Y_\tau = -Y F(T) + \dfrac{mP_0}{LeRC_p}\dfrac{\lambda}{T}(Y_\xi)_\xi \ , \end{cases} \tag{1.41}$$

$$\begin{cases} \rho RT = mP_0 \ , \\ mP_0 u_\xi = RT_\tau \ , \\ p_\xi = u_\tau \ . \end{cases} \tag{1.42}$$

It should be emphasized here that the use of the Lagrangian coordinate (1.32) uncouples the equations (1.41) for the "combustion variables" T and Y (which take the form of a purely diffusive reactive system) from the equations (1.42) for the "hydrodynamical variables" ρ, u and p.

The systems (1.28) and (1.41)-(1.42) are investigated from a rigorous mathematical point of view in Chapter 2; the numerical study of their solutions is discussed in Chapter 4.

2.2. Thermo-diffusive approximation

We have observed that the reaction-diffusion and the hydrodynamical effects are decoupled in the isobaric model (1.20) in the one-dimensional case, both for steady and unsteady solutions. This decoupling no longer appears in higher dimensions. This is the reason why the physicists have introduced an additional approximation, *the constant density approximation*, which consists in neglecting also the density fluctuations in the mixture (see Barenblatt et al [9], Sivashinsky [127]). This approximation is more drastic than the isobaric simplification, and more delicate to justify from a physical point of view; but it leads to a simpler model in which a decoupling again appears, which has allowed numerous improvements in the understanding of flame propagation phenomena. This model is essentially valid for situations where the hydrodynamical effects play a secondary role with respect to the reactive and diffusive effects, in other words, when the gas flow is not too far from being uniform. Let us finally mention that this essentially qualitative model retains many features of flame propagation phenomena, including cellular flame instabilities, and formally leads (using the well-known asymptotics for high activation energies) to the Kuramoto-Sivashinsky equation for the evolution of the flame front (see Chapter 5).

In the framework of the constant-density approximation, the equations (1.20) become:

$$\rho = Constant \ , \tag{1.43}$$

(which is the "new equation of state"),

$$\begin{cases} u_x + v_y = 0 \ , \\ \rho u_t + \rho u u_x + \rho v u_y = -p_x \ , \\ \rho v_t + \rho u v_x + \rho v v_y = -p_y \ , \end{cases} \tag{1.44}$$

and:

$$\begin{cases} \rho C_p T_t + \rho C_p u T_x + \rho C_p v T_y = Q\rho Y F(T) + \vec{\nabla}.(\lambda \vec{\nabla} T) , \\ \rho Y_t + \rho u Y_x + \rho v Y_y = -\rho Y F(T) + \vec{\nabla}.(\rho D \vec{\nabla} Y) . \end{cases} \tag{1.45}$$

The "combustion variables" no longer appear in the system (1.43)-(1.44) describing the behaviour of the "hydrodynamical variables" u, v, p. If one is interested in the flame structure, that is in the temperature and mass fraction fields, one may therefore consider the system (1.45) while assuming that the velocity (u, v) is given and satisfies (1.44). For the case of a flame propagating in the infinite rectangular channel S, it is natural to choose a velocity field parallel to the tube walls: $v \equiv 0$; (1.45) then takes the form:

$$\begin{cases} C_p T_t + C_p u T_x = QY F(T) + \rho^{-1} \vec{\nabla}.(\lambda \vec{\nabla} T) , \\ Y_t + u Y_x = -Y F(T) + \rho^{-1} \vec{\nabla}.(\rho D \vec{\nabla} Y) \quad \text{in } S = \mathbb{R} \times (0, L) . \end{cases} \tag{1.46}$$

These equations are associated to initial data, and to boundary conditions of the form:

$$\begin{cases} T(-\infty, y, t) = T_u , \quad Y(-\infty, y, t) = Y_u , \\ T(+\infty, y, t) = T_b , \quad Y(+\infty, y, t) = 0 \quad \text{for } y \in (0, L) \quad \text{and } t \geq 0 , \end{cases} \tag{1.47}$$

at both ends of the tube, and

$$\begin{cases} T_y(x, 0, t) = T_y(x, L, t) = 0 , \\ Y_y(x, 0, t) = Y_y(x, L, t) = 0 , \quad \text{for } x \in \mathbb{R} \quad \text{and } t \geq 0 , \end{cases} \tag{1.48}$$

in the case of adiabatic, non catalytic walls. The mathematical and numerical investigation of this model, known in combustion theory as the unsteady *thermo-diffusive* model, is presented in Chapter 5 in the case where $u = Constant$.

When the Lewis number Le is equal to unity, it is easy to check that any *steady* solution of (1.46) satisfies the identity $QY = C_p(T_b - T)$. This solution is then given by a system containing only one partial differential equation, which can be written in the following normalized form (notice that (1.44) yields $u = u(y)$ for a steady solution):

$$\begin{cases} -\Delta\Theta + u(y)\Theta_x = g(\Theta) \quad \text{in } S = \mathbb{R} \times (0, L) , \\ \Theta(-\infty, y) = 0 , \quad \Theta(+\infty, y) = 1 \quad \text{for } y \in (0, L) , \\ \Theta_y(x, 0) = \Theta_y(x, L) = 0 \quad \text{for } x \in \mathbb{R} . \end{cases} \tag{1.49}$$

Some mathematical results concerning this two-dimensional elliptic problem set in the infinite strip S are presented in Chapter 3.

3. PREMIXED FLAME PROPAGATION

3.1. Introduction

Before presenting the mathematical and numerical investigation of the above models, we feel necessary to briefly describe from a physical point of view how a flame propagates inside a gaseous mixture. We are going to do this by considering the simple case of a planar (one-dimensional) steady flame.

The simplest way of describing this flame, i.e. of describing the solutions of (1.26)-(1.27), is to use the classical "high activation energy limit". The analysis therefore relies on the fact that, in actual problems, the activation energy $\mathcal{E}$ is large compared to the values of the product RT in the considered range of temperature: the Arrhenius term $e^{-\mathcal{E}/RT}$ is then highly nonlinear. This fact has been intensively used by the physicists to analyse flame propagation, since the pioneer work of Zeldovich and Frank-Kamenetskii [154], and especially in the last fifteen years (see e.g. Buckmaster-Ludford [36], Clavin [40], Clavin-Liñan [41], Sivashinsky [127]).

In the framework of the high activation energy limit, the structure of the planar steady flame is derived using *matched asymptotic expansions* (see e.g. Buckmaster-Ludford [36], Clavin-Liñan [41], Joulin-Clavin [78] and [93]). But we find it simpler and more instructive to follow here a more physical (and less rigorous) approach, in which we simply use physical arguments to determine which terms of the governing equations are dominant and which terms on the opposite are negligible.

For those readers who might be tempted to skip over this section because of the announced lack of mathematical rigor in the forthcoming analysis, let us already point out that this analysis for high activation energies will appear in the next chapter to be completely justified from a mathematical point of view, and that they are strongly encouraged to follow the elementary physical analysis presented below!

3.2. The analysis for high activation energies

To simplify the analysis, we consider a planar steady flame with a Lewis number equal to unity: $Le = 1$. It it then easy to see that any solution (c, Θ, Z) of (1.26)-(1.27)

satisfies $\Theta + Z = 1$. We are then left with a single equation:

$$\begin{cases} -\Theta_{xx} + c\Theta_x = g(\Theta) \text{ on } \mathbb{R}\,, \\ \Theta(-\infty) = 0\,, \quad \Theta(+\infty) = 1\,, \end{cases} \tag{1.50}$$

where both the function Θ and the real c are unknown (we have substituted x for x' and we have set $g(s) = f(s)(1-s)$). Assuming for simplicity that the temperature dependance of the reaction term is only given by the Arrhenius exponential factor $e^{-\mathcal{E}/RT}$ (with $T = T_u + \Theta(T_b - T_u)$), we use the identity:

$$\exp\left(-\frac{\mathcal{E}}{RT}\right) = \exp\left(-\frac{\mathcal{E}}{RT_b}\right).\exp\left(\frac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right)\,, \tag{1.51}$$

where $\beta = \dfrac{\mathcal{E}}{RT_b}\dfrac{T_b - T_u}{T_b} > 0$ is the reduced activation energy (also called the Zeldovich number), and $\alpha = \dfrac{T_b - T_u}{T_b} > 0$ is a nondimensional heat release parameter, and rewrite (1.50) as:

$$\begin{cases} -\Theta'' + c\Theta' = K(1-\Theta)\exp\left(\dfrac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right) = g_\beta(\Theta) \text{ on } \mathbb{R}\,, \\ \Theta(-\infty) = 0\,, \quad \Theta(+\infty) = 1\,, \end{cases} \tag{1.52}$$

with $K > 0$.

We therefore want to describe the solution (c, Θ) of (1.52) for large values of the activation energy, i.e. in the limit $\beta \to +\infty$. The basic remarks are the following:

(i) for β large, the function $\exp\left(\dfrac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right)$ essentially behaves as $\exp(-\beta(1-\Theta))$, and is therefore negligible compared to 1 (its value for $\Theta = 1$), except in the region where $1 - \Theta \simeq O(\beta^{-1})$, let us say where:

$$1 - \frac{\kappa}{\beta} \leq \Theta < 1\,, \tag{1.53}$$

with $\kappa = O(1)$;

(ii) we admit (from experimental evidence) that this region where the reaction term is significantly large, hereafter called the reaction zone, is localized in a bounded interval $[x_1, x_2]$ of $\mathbb{R}$;

(iii) we also assume that the mass flux c remains of order $O(1)$ when $\beta \to +\infty$.

As a consequence, we assume that the reaction rate can be neglected outside the reaction zone $[x_1, x_2]$. We have there:

$$-\Theta'' + c\Theta' = 0\,, \tag{1.54}$$

whence $\Theta = a + b\exp(cx)$ for some constants a and b. Using (1.53) and the boundary conditions in (1.52), we get:

$$\Theta(x) = (1 - \frac{\kappa}{\beta})\exp[c(x - x_1)] \quad \text{for } x \leq x_1 \tag{1.55}$$

in the fresh mixture ahead of the reaction zone, and:

$$\Theta = 1 \quad \text{for } x \geq x_2 \tag{1.56}$$

in the burnt gases, behind the reaction zone. It can be noticed here that (1.55) could also be written as $\Theta = \exp(cx)$ with an appropriate choice of the origin.

Let us now evaluate the reaction zone thickness. From (1.53), the variation of temperature inside this zone is $\Delta\Theta \simeq \kappa\beta^{-1}$. At the left extremity of this zone (for $x = x_1$), the temperature gradient is:

$$\Theta_x(x_1) = c\Theta(x_1) = c + O(\beta^{-1}) \tag{1.57}$$

from (1.55); in the same way, the temperature gradient at the right extremity of this zone is (in first approximation):

$$\Theta_x(x_2) = 0 \tag{1.58}$$

from (1.56). Then an average value of the temperature gradient inside the reaction zone is:

$$\bar{\Theta}_x = \frac{c}{2} + O(\beta^{-1})\,, \tag{1.59}$$

and we can evaluate the reaction zone thickness $x_2 - x_1$ by writing:

$$x_2 - x_1 = \frac{\Delta\Theta}{\bar{\Theta}_x} = \frac{1}{c}\frac{2\kappa}{\beta} + O(\beta^{-2})\,. \tag{1.60}$$

Then, the reaction zone becomes infinitely thin when β tends to $+\infty$. In the limit, the reaction is localized at one point $x = \tilde{x}$, and we have:

$$\Theta(x) = \begin{cases} \exp[c(x - \tilde{x})] & \text{for } x \leq \tilde{x}\,, \\ 1 & \text{for } x \geq \tilde{x}\,. \end{cases} \tag{1.61}$$

It is interesting to notice here that the limiting solution Θ given by (1.61) satisfies:

$$\begin{cases} -\Theta'' + c\Theta' = c\delta_{\tilde{x}} , \\ \Theta(-\infty) = 0 , \quad \Theta(+\infty) = 1 ; \end{cases} \tag{1.62}$$

thus, in the limit $\beta \to +\infty$, the reaction term $g_\beta(\Theta)$ tends to a Dirac delta function located at some point $x = \tilde{x}$.

The solution of (1.52) would then be completely determined in the limit $\beta \to +\infty$ if the value of c were known. Evaluating this value requires an internal analysis of the thin reaction zone.

To do this analysis, we need to evaluate an average value of the second derivative of the temperature inside the reaction zone. Using (1.57), (1.58) and (1.60), we have:

$$\bar{\Theta}_{xx} = \frac{\Theta_x(x_2) - \Theta_x(x_1)}{x_2 - x_1} = -\beta\frac{c^2}{2\kappa} + O(1) . \tag{1.63}$$

Comparing (1.59) and (1.63), we see that, inside the reaction zone, the first derivative Θ_x is negligible compared to the second derivative Θ_{xx}; we will then consider that the temperature satisfies inside the reaction zone the equation:

$$-\Theta'' = g_\beta(\Theta) . \tag{1.64}$$

Multiplying this equation by $2\Theta'$ and integrating over the whole reaction zone, we get:

$$-\int_{x_1}^{x_2} \frac{d}{dx}[(\Theta')^2]dx = 2\int_{\Theta(x_1)}^{\Theta(x_2)} g_\beta(\Theta)d\Theta , \tag{1.65}$$

whence, from (1.56)-(1.58):

$$c^2 = 2\int_{\Theta(x_1)}^{1} g_\beta(\Theta)d\Theta . \tag{1.66}$$

Since (by definition of x_1) we have considered that the reaction term $g_\beta(\Theta)$ is negligible for $\Theta \leq \Theta(x_1)$, we may modify the lower bound for the integral in the right-hand side of (1.66). We can finally write:

$$c = \sqrt{2\int_0^1 g_\beta(\Theta)d\Theta} , \tag{1.67}$$

which gives the value of c and achieves the analysis: in the limit $\beta \to +\infty$, the solution (c, Θ) of (1.52) is given by (1.62) and (1.67).

3.3. The structure of the steady planar flame

The same analysis can be carried out in the more general case where the Lewis number is non necessarily unity, leading also to the steady planar flame structure shown on Figure 1.1 below, where one can basically observe three different regions:

(i) the fresh mixture, where $\Theta \approx 0$, $Z \approx 1$;

(ii) the burnt gases, where $\Theta \approx 1$, $Z \approx 0$;

(iii) and, between these two regions, the *flame*, that is the region (whose thickness L_f is of the order of c^{-1} from (1.55)) where the temperature and mass fraction variations occur. The flame can itself be divided into two smaller zones:

* the pre-heat zone, of thickness L_f, where convection and diffusion balance each other (see (1.54)), and where the temperature profile is exponential;

* and the reaction zone, whose thickness $x_2 - x_1$ is of the order of $2\beta^{-1}L_f$ from (1.60), where diffusion and reaction balance each other (see (1.64)).

Figure 1.1: Structure of a steady planar premixed flame.

Insert Figure 1.1

It should be noticed here that the reaction rate is negligibly small everywhere outside the reaction zone, but for two mainly different reasons: in the hot gases, there is no chemical reaction because there is nothing to burn ($Z = 0$), whereas, in the fresh mixture and in the pre-heat zone, the reaction does not take place at a significant rate only because the mixture is too cold.

The flame we have considered is steady in a reference frame where the mass flux is constant $\rho u = c$ (see (1.21)), and therefore where the fresh mixture at $-\infty$ has a positive velocity $u(-\infty) = c\rho(-\infty)^{-1} = V_f$. The same flame could also be observed in a reference frame where the fresh mixture at $-\infty$ is at rest; the flame then propagates towards the fresh gases, at the velocity $-V_f$. The mechanism of this propagation now

clearly appears: the burnt gases being hot, the heat released inside the thin reaction zone by the exothermic chemical reaction diffuses forward, towards the fresh gases; the temperature of those slices of the mixture which are located just ahead of the reaction zone increases because of this diffusive heat flux, so that they eventually react in turn. This description shows that the mechanism of laminar flame propagation is controlled by the balance between convection and diffusion in the pre-heat zone, and the balance between diffusion and reaction in the reaction zone.

Remark 1.3: Let us finally express the result (1.67) for the reaction term g_β given by the Arrhenius law in (1.52); we get:

$$c^2 = 2\int_0^1 g_\beta(\Theta)d\Theta = \frac{2K}{\beta^2}\ , \tag{1.68}$$

which shows that the preceding physical analysis is meaningful only if the Arrhenius prefactor K behaves as β^2. More precisely, the analysis presented in Section 3.2 shows that the solution (c,Θ) of:

$$\begin{cases} -\Theta'' + c\Theta' = \dfrac{\beta^2}{2}(1-\Theta)\exp\left(\dfrac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right) & \text{on } \mathbb{R}\ , \\ \Theta(-\infty) = 0\ ,\quad \Theta(+\infty) = 1\ , \end{cases} \tag{1.69}$$

tends in the limit $\beta \to +\infty$ towards (c_0,Θ_0) given by $c_0 = 1$ and:

$$\begin{cases} -\Theta_0'' + c_0\Theta_0' = c_0\delta_{\frac{1}{2}}\ , \\ \Theta_0(-\infty) = 0\ ,\quad \Theta_0(+\infty) = 1\ . \end{cases} \tag{1.70}$$

This result can be extended to the case $Le \neq 1$; one easily shows, using similar arguments, that the solution (c,Θ,Z) of:

$$\begin{cases} -\Theta'' + c\Theta' = \dfrac{\beta^2}{2Le}Z\exp\left(\dfrac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right)\ , \\ -\dfrac{1}{Le}Z'' + cZ' = -\dfrac{\beta^2}{2Le}Z\exp\left(\dfrac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right) & \text{on } \mathbb{R}\ , \\ \Theta(-\infty) = 0\ ,\quad \Theta(+\infty) = 1\ , \\ Z(-\infty) = 1\ ,\quad Z(+\infty) = 0\ , \end{cases} \tag{1.71}$$

tends in the limit $\beta \to +\infty$ towards (c_0,Θ_0,Z_0) given by $c_0 = 1$ and:

$$\begin{cases} -\Theta_0'' + c_0\Theta_0' = c_0\delta_{\frac{1}{2}}\ , \\ -\dfrac{1}{Le}Z_0'' + c_0Z_0' = -c_0\delta_{\frac{1}{2}}\ , \\ \Theta_0(-\infty) = 0\ ,\quad \Theta_0(+\infty) = 1\ . \\ Z_0(-\infty) = 1\ ,\quad Z_0(+\infty) = 0\ . \end{cases} \tag{1.72}$$

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