PLANE LAMINAR FLAMES WITH MULTICOMPONENT TRANSPORT AND COMPLEX CHEMISTRY

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We consider plane laminar flames with multicomponent transport and complex chemistry. The governing equations are derived from the kinetic theory of gases by using the classical isobaric approximation. An arbitrary number of reversible chemical reactions and temperature dependent species specific heats are considered in the model. The most general form for multicomponent transport fluxes given by the kinetic theory is also taken into account. Upon first considering a bounded domain and then letting the size of the domain to go to infinity, we obtain an existence theorem. We also establish that the natural entropy production norm associated with multicomponent diffusion is a solution–weighted norm.

1. INTRODUCTION

Numerous studies have recently been devoted to plane laminar flames with complex chemistry [Hei87] [VV90] [Bon92] [BL93] [VV94] [Bon94]. Important advances have been made in these papers which were essentially concerned with irreversible exothermic chemical reaction networks and elementary transport models.

In this work, we investigate the flame equations derived from the kinetic theory of dilute polyatomic reactive gas mixtures [EG94]. The reaction network that we consider is composed of an arbitrary number of reversible chemical reactions. The reaction rates of progress are of Maxwellian type and the rate contants satisfy natural reciprocity relations. Moreover, the most general form for multicomponent transport fluxes obtained from the kinetic theory is included in the model with mixture dependent transport coefficients. In particular, all species second derivatives are coupled through diffusive processes and are coupled to the temperature second derivatives through thermal diffusion, that is, species diffusion due to temperature gradients. The temperature dependence of species specific heats is also taken into account.

We consider two types of cold boundary conditions. The first type is associated with the anchored flame model [HCC53] and the corresponding domain is the half line $[0, \infty)$. This model also corresponds to boundary conditions often used in numerical simulations of complex chemistry flames [Ser86] [GS92]. It also modelizes an experimental configuration where the flame is dynamically stabilized far away from the injection device by using laser tomography [Qal84] [Cla85]. The second type of boundary conditions that we consider is that of an infinitly far cold boundary. The corresponding domain is then the full line $(-\infty, \infty)$. In this situation, we use a Heavyside cutoff function for the source term in order to remove the cold boundary difficulty and both models are shown to be equivalent. On the other hand, the hot boundary condition is of Dirichlet type and corresponds to an equilibirum point whose existence and uniqueness is established.

We first consider the problem on a bounded domain $[0, a]$. The existence theorem is obtained by using a fixed point formulation and the Leray-Schauder topological degree. The definition of the degree is obtained by estimating a priori the solutions. In particular, we obtain for the first time an estimate of the maximum temperature in a flame with nontrivial transport. To this purpose, we establish a fundamental inequality for the quadratic form associated with diffusion matrices, using previous results on multicomponent transport [Gio91] [EG94]. Combining this inequality with the entropy conservation equation, we obtain a natural entropy production norm for diffusive processes which is a solution–weighted norm in the form

$$\sum_{k \in S} \int \frac{\partial_{\boldsymbol{x}} Y_k \cdot \partial_{\boldsymbol{x}} Y_k}{Y_k} \, dx,$$

where Y_k is the mass fraction of the k^{th} species and S the set of species indices.

We then let $a \to \infty$ and obtain an existence theorem as well as exponential convergence towards equilibrium at infinity. A key point in the proof is to derive a lower bound independent of a for the eigenvalue of the flame problem. Exponential convergence towards equilibrium is achieved by using entropic estimates and a stability inequality concerning the chemical dissipation rate.

The governing equations for complex chemistry flames are presented in Section 2. In Section 3 we specify the mathematical properties for thermodynamic functions and we establish existence and uniqueness of the equilibrium state at the hot boundary. The mathematical properties of transport coefficients are investigated in Section 4 where we establish the fundamental diffusion inequality and the entropy conservation equation. The equivalence of both problem formulations is obtained in Section 5. Existence on a bounded domain is obtained in Section 6 and, finally, existence of a solution is obtained in Section 7.

2. GOVERNING EQUATIONS

The governing equations for steady plane laminar flames with complex chemistry and detailed transport are obtained from the multicomponent reactive flow equations—derived from the kinetic theory—under the classical isobaric approximation.

2.1. Conservation equations

The equations modeling steady plane laminar flames with complex chemistry express the conservation of species mass and energy. The species conservation equations can be written in the form [Wil85] [EG94]

$$c\,Y_k' + \mathcal{F}_k' = m_k \omega_k, \qquad k \in S, \tag{2.1}$$

where c is the mass flow rate, Y_k the mass fraction of the k^{th} species, "$\,'\,$" the space derivative operator, $\mathcal{F}_k$ the mass flux of the k^{th} species, m_k the molar mass of the k^{th} species, ω_k the molar production of the k^{th} species, $S = [1, n]$ the set of species indices and n the number of species assumed to be $n \geq 2$.

The energy conservation equation can be written in the enthalpy form

$$c\,h' + q' = 0, \tag{2.2}$$

where h is the specific enthalpy of the mixture and q the heat flux. By using the expressions of the mixture enthalpy h and of the heat flux q, a governing equation for the absolute temperature T will be obtained in Section 2.6.

The unknowns are the mass flow rate c, which is a nonlinear eigenvalue of the problem, the mass fraction vector $Y = (Y_1, \ldots, Y_n)^\star$ where * is the transposition symbol, and the enthalpy h—or equivalently the absolute temperature T. It will be convenient to introduce the unknown ξ defined by

$$\xi = (h,\, Y_1, \ldots,\, Y_n)^\star. \tag{2.3}$$

The corresponding fluxes are denoted by

$$\phi = (q,\, \mathcal{F}_1, \ldots,\, \mathcal{F}_n)^\star, \tag{2.4}$$

and the corresponding sources by

$$w = (0,\, m_1\omega_1, \ldots,\, m_n\omega_n)^\star. \tag{2.5}$$

The conservation equations can then be written in the compact form

$$c\,\xi' + \phi' = w, \tag{2.6}$$

and these equations have to be completed by the relations expressing the transport fluxes $\mathcal{F}_k$, $k \in S$, and q, the thermodynamic properties like the enthalpy h, and the chemical source terms ω_k, $k \in S$.

2.2. Thermodynamic properties

The pressure p is taken to be a positive constant

$$p = \text{Cte}, \tag{2.7}$$

and the density is given by the state law

$$\rho(T, Y) = \frac{p}{RT}\Big(\sum_{k\in S}\frac{Y_k}{m_k}\Big)^{-1}, \tag{2.8}$$

where R the universal gas constant and T the absolute temperature. The specific internal enthalpy h of the mixture is given by the expression

$$h(T, Y) = \sum_{k\in S} Y_k h_k(T), \tag{2.9}$$

where the quantity h_k is the internal energy per unit mass of the k^{th} species. The quantity $h_k = h_k(T)$ can be written

$$h_k(T) = h_k^0 + \int_{T_0}^{T} c_{pk}(t)\ dt, \tag{2.10}$$

where h_k^0 is the enthalpy of formation of the k^{th} species at the positive reference temperature T_0 and c_{pk} is the specific heat at constant pressure of the k^{th} species. The mixture specific heat at constant pressure c_p is defined similarly by

$$c_p(T, Y) = \sum_{k\in S} Y_k c_{pk}(T). \tag{2.11}$$

The mathematical assumptions concerning the specific heats c_{pk}, $k \in S$, are specified in Section 3.

Species mole fractions are also needed for modeling complex chemistry flames. Indeed, although mass related quantities like momentum are conserved during molecular collisions, chemistry production rates and diffusive processes are related to species collision rates, and therefore, to molar properties. We denote by X_k the mole fraction of the k^{th} species defined by

$$X_k(Y) = \frac{\overline{m}}{m_k}\ Y_k, \tag{2.12}$$

where $\overline{m}$ is the molar mass of the mixture given by

$$\frac{\sum_{k\in S} Y_k}{\overline{m}} = \sum_{k\in S}\frac{Y_k}{m_k}. \tag{2.13}$$

In the following, we will also need the quantity γ_k defined by

$$\gamma_k = \frac{Y_k/m_k}{\sum_{l\in S} Y_l/m_l} = \frac{X_k}{\sum_{l\in S} X_l} \tag{2.14}$$

and which essentially represents the mole fraction of the k^{th} species.

The natural species variables for flame problems are the mass fractions. We have chosen, for convenience, to consider these mass fractions Y_k, $k \in S$, as formally independent unknowns, and to recover the relation $\sum_{k\in S} Y_k = 1$ from the conservation equations. As a consequence, some care must be taken in defining thermodynamic properties, in order to maintain homogeneity and extensivity. In particular, the relation (2.13) contains a factor $\sum_{k\in S} Y_k$ which avoids various artificial singularities, e.g., when relating the derivatives of mole and mass fractions [Gio90] [Gio91]. After some algebra, the relations (2.12) (2.13) yields that $\sum_{k\in S} Y_k = \sum_{k\in S} X_k$ so that we also recover the relation $\sum_{k\in S} X_k = 1$ from the species equations.

2.3. Thermodynamic properties for positive mass fractions

The thermodynamic properties introduced in Section 2.2 are defined for nonnegative nonzero mass fractions $Y \geq 0$, $Y \neq 0$. We write $z \geq 0$, respectively $z > 0$, when $z = (z_1, \dots, z_n)$ and $z_k \geq 0$, respectively $z_k > 0$, for every $k \in S$. For positive mass fractions $Y > 0$, however, we can further define the species entropies and free enthalpies. Indeed, the kinetic theory yields the specific entropy of the k^{th} species

$$s_k(T, Y) = s_k^{0p} + \int_{T_0}^{T} \frac{c_{pk}(t)}{t}\, dt - \frac{R}{m_k} \log(\gamma_k), \tag{2.15}$$

where s_k^{0p} the formation entropy of the k^{th} species at the positive reference temperature T_0 and pressure p. It will be convenient to define

$$s_k^p(T) = s_k^{0p} + \int_{T_0}^{T} \frac{c_{pk}(t)}{t}\, dt \tag{2.16}$$

which represents the entropy of the k^{th} species at pressure p. The specific entropy of the mixture is then the quantity

$$s(T, Y) = \sum_{k\in S} Y_k s_k(T, Y), \tag{2.17}$$

and will play a fundamental role in the analysis.

We will also need the expression of the species free enthalpies g_k, $k \in S$, that is, the species Gibbs functions

$$g_k(T, Y) = h_k(T) - s_k(T, Y)\, T, \tag{2.18}$$

and the standard free enthalpy g_k^p at pressure p

$$g_k^p(T) = h_k(T) - s_k^p(T)\, T. \tag{2.19}$$

Finally, we introduce for convenience the reduced quantities

$$\mu_k^p(T) = \frac{g_k^p(T)}{RT}, \qquad \mu_k(T, Y) = \frac{g_k}{RT} = \mu_k^p(T) + \frac{1}{m_k} \log(\gamma_k), \tag{2.20}$$

The free enthalpies g_k, $k \in S$, and the quantities μ_k, $k \in S$, will be needed for investigating chemical equilibrium and the entropy production rate due to chemistry.

2.4. Maxwellian chemistry

We consider a system of n_R reversible reactions for n species

$$\sum_{k\in S} \nu_{ki}^{\mathrm{d}} \mathcal{S}_k \rightleftharpoons \sum_{k\in S} \nu_{ki}^{\mathrm{r}} \mathcal{S}_k, \qquad i \in R, \tag{2.21}$$

where $\mathcal{S}_k$ is the chemical symbol of the k^{th} species, ν_{ki}^{d} and ν_{ki}^{r} the direct and reverse stoichiometric coefficients of the k^{th} species in the i^{th} reaction, and $R = [1, n_R]$ the set of reaction indices. Note that all chemical reactions are reversible and that the number of reactions n_R is arbitrary.

The molar production rates that we consider are the Maxwellian production rates obtained from the kinetic theory [EG94]. These rates are obtained in a reactive kinetic framework—when the chemistry characteristic times are larger than the mean free times of the molecules—and are compatible with the law of mass action [EG94]. In this situation the molar production rate of the k^{th} species can be written in the form [Wil85] [EG94]

$$\omega_k = \sum_{i\in R} \nu_{ki}\, r_i, \tag{2.22}$$

where

$$\nu_{ki} = \nu_{ki}^{\mathrm{r}} - \nu_{ki}^{\mathrm{d}}, \tag{2.23}$$

and where r_i is the rate of progress of the i^{th} reaction. This rate r_i is given by

$$r_i = K_i^{\mathrm{d}} \prod_{k\in S} \gamma_k^{\nu_{ki}^{\mathrm{d}}} - K_i^{\mathrm{r}} \prod_{k\in S} \gamma_k^{\nu_{ki}^{\mathrm{r}}}, \tag{2.24}$$

where γ_k is given by (2.14) and K_i^{d} and K_i^{r} are the direct and reverse rate constants of the i^{th} reaction. Note that the reaction rates of progress are usually expressed in terms of species concentrations $\rho Y_k/m_k$, $k \in S$, rather than in terms of the γ_k, $k \in S$. However, the expressions (2.24) are more suited to flame problems and are easily obtained, after a little algebra, making use of the state law and of the isobaric approximation. On the other hand, the quantities K_i^{d} and K_i^{r} are functions of the temperature and their ratio is the equilibrium constant K_i^{e} of the i^{th} reaction

$$K_i^{\mathrm{e}}(T) = \frac{K_i^{\mathrm{d}}(T)}{K_i^{\mathrm{r}}(T)}, \tag{2.25}$$

given by

$$\log K_i^{\mathrm{e}}(T) = -\sum_{k\in S} \frac{\nu_{ki} m_k}{R}\, \frac{g_k^p(T)}{T}, \tag{2.26}$$

where $g_k^p(T)$ is defined by (2.19).

The mathematical properties of the chemical source terms will be specified in section 3. In particular, the stoichiometric coefficients satisfy element conservation and total mass conservation.

There are several reasons for considereing only reversible chemical reactions in the network. Indeed, the macroscopic constants K_i^{d} and K_i^{r} are Maxwellian averaged values of molecular chemical cross sections appearing in reactive collisional source terms of the species Boltzmann equations [EG94]. However, direct and reverse chemical cross sections are always proportional, as are non reactive cross sections in any Boltzmann equation, as can be shown from quantum mechanics [EG94]. A direct consequence is the fundamental proportionality relation between the macroscopic direct and reverse rate constants $K_i^{\mathrm{d}}(T) = K_i^{\mathrm{r}}(T)/K_i^{\mathrm{e}}(T)$ [EG94]. Consequently, we cannot assume that one reaction constant vanishes without assuming that both vanish. A second reason for assuming full reversibility is that the model must be able to describe the equilibrium mixture at the hot boundary. However, statistical mechanics for uniform mixtures at equilibrium also shows that detailed balance must prevail, so that irreversibility again cannot be assumed. Last, but not least, hundreds of experimental measurements have shown the validity of the fundamental relation $K_i^{\mathrm{d}}(T) = K_i^{\mathrm{r}}(T)/K_i^{\mathrm{e}}(T)$. Note also the difference between (2.24) and the rates of progress considered in previous studies where the mass fractions appear in place of the mole fractions. This shows that the assumption $m_k = \overline{m}$, $k \in S$, has implicitly been made in all previous studies unlike the present paper where the distinction between mass and mole properties is kept.

Remark 2.1. Another formalism for describing chemical networks has been introduced by Feinberg [Fei95]. In Feinberg's formalism, it is possible to associate an integer, named the default, to each reaction network. In this formalism, only "zero default" reaction networks have a satisfactory behavior for *all* possible values of the rate constants. In Feinberg's formalism, however, direct and reverse constants are assumed to be independent. Feinberg's negative results thus concern networks for which the ratio $K_i^{\mathrm{d}}(T)/K_i^{\mathrm{r}}(T)$ is arbitrary. This is not the case according to the kinetic theory which yields the fundamental constraint $K_i^{\mathrm{d}}(T) = K_i^{\mathrm{r}}(T)/K_i^{\mathrm{e}}(T)$. In particular, this relation can be interpreted as a natural *compatibility condition* between chemistry and thermodynamics. When this fundamental relation is assumed to hold, all classical results from thermochemistry are valid [SS65] [Kra87] and there are strictly no restrictions on the number of chemical reactions—other than obvious combinatorics—or on their linear dependency. In this situation, Feinberg's default can be *arbitrarily large*, but the corresponding networks have a very satisfactory behavior and can be naturally investigated by using Gibbs classical thermochemistry [SS65] [Kra70] [GM98] ■

Remark 2.2. The direct rate constant is usually approximated by using a generalized Arrhenius empirical relation

$$K_i^{\mathrm{d}}(T) = \mathfrak{A}_i T^{\mathfrak{b}_i} \exp\Big(-\frac{\mathfrak{E}_i}{RT}\Big),$$

where $\mathfrak{A}_i > 0$ is the pre-exponential factor, $\mathfrak{b}_i$ the pre-exponential exponent and $\mathfrak{E}_i \geq 0$ the activation energy of the i^{th} reaction, but the exact expression of $K_i^{\mathrm{d}}(T)$ will not be needed in the following. Note that these expressions are not bounded for large T when $\mathfrak{b}_i$ is positive. ■

2.5. Transport fluxes

The expressions for transport fluxes are obtained from the kinetic theory of dilute polyatomic gas mixtures. We first express these fluxes in the general situation of nonnegative mass fractions, that is, when $Y \geq 0$, $Y \neq 0$. Such a dictinction between positive and nonnegative mass fractions naturally arises in the kinetic theory of dilute polyatomic gas mixtures [Gio91] [EG94].

Under the isobaric approximation, the species fluxes $\mathcal{F}_k$, $k \in S$, and the heat flux q are in the form

$$\mathcal{F}_k = -\sum_{l \in S} C_{kl}\big(\gamma_l' + \gamma_l \widetilde{\chi}_l (T'/T)\big), \qquad k \in S, \tag{2.27}$$

$$q = \ -\lambda T' + RT \sum_{l \in S} (\widetilde{\chi}_l / m_l)\mathcal{F}_l + \sum_{l \in S} h_l \mathcal{F}_l, \tag{2.28}$$

where $C = (C_{kl})_{k,l \in S}$ is the flux diffusion matrix, γ_k the quantity given in (2.14), $\widetilde{\chi} = (\widetilde{\chi}_1, \ldots, \widetilde{\chi}_n)^\star$ the rescaled thermal diffusion ratios, and λ the thermal conductivity.

For positive mass fractions, one can further introduce the species diffusion velocities V_k, $k \in S$, defined by

$$V_k = \frac{\mathcal{F}_k}{\rho Y_k}, \tag{2.29}$$

and from (2.27), one can express these velocities as

$$V_k - \sum_{l \in S} D_{kl}\big(\gamma_l' + \gamma_l \widetilde{\chi}_l (T'/T)\big), \qquad k \in S, \tag{2.30}$$

where $D = (D_{kl})_{k,l \in S}$ is the diffusion matrix defined by $D_{kl} = C_{kl}/(\rho Y_k)$, $k, l \in S$. The diffusion velocities turn out to be of fundamental importance since the matrix D is symmetric positive semi-definite and is the matrix associated with entropy production as will be shown in Section 4. Note that the multicomponent fluxes that we use have natural symmetry properties [WT62] [FK72] [Gio91] [EG94] which have artificially been destroyed in [HCB54].

Remark 2.3. The kinetic theory specifically yields Equation (2.27) with p_k'/p in place of γ_k', where $p_k = \rho RT Y_k / m_k = p\gamma_k$ is the partial pressure of the k^{th} species [EG94]. However, from the isobaric approximation, we have $p_k'/p = (p_k/p)' = \gamma_k'$. ■

Alternate expressions for the diffusion velocities and the heat flux vector are

$$\mathcal{F}_k = -\sum_{l \in S} C_{kl}\gamma_l' - \rho Y_k \theta_k (T'/T), \qquad k \in S, \tag{2.31}$$

$$q = \ -\widehat{\lambda} T' - p \sum_{k \in S} \theta_k \gamma_k' + \sum_{k \in S} h_k \mathcal{F}_k, \tag{2.32}$$

where $\theta = (\theta_1, \ldots, \theta_n)^\star$ are the thermal diffusion coefficients, and $\widehat{\lambda}$ the partial thermal conductivity. These expressions are more classical than (2.27) (2.28) and lead to Onsager reciprocal relations. However, the expressions (2.27) (2.28) are more practical from a mathematical point of view.

Note that all species second derivatives are coupled through the flux diffusion coefficients C and that multicomponent fluxes naturally involve mole fractions derivatives. In addition, species and temperature derivatives are coupled through the thermal diffusion coefficients $\widetilde{\chi}$. These effects were not previously considered in flame models.

The mathematical properties of the transport coefficients λ, C, D, and $\widetilde{\chi}$ are specified in section 4.

2.6. The temperature equation

In order to derive a governing equation for the absolute temperature T, we can use equations (2.1) (2.2) and the definition of the mixture enthalpy h. After a little algebra, we easily obtain that

$$c_p T' = -\big(q - \sum_{k\in S} h_k \mathcal{F}_k\big)' - \sum_{k\in S} c_{pk} T' \mathcal{F}_k - \sum_{k\in S} h_k m_k \omega_k. \tag{2.33}$$

Using now the expression (2.28) for the heat flux q, we finally obtain the temperature equation

$$c\, c_p T' = \big(\lambda T' - RT \sum_{l\in S} (\widetilde{\chi}_l/m_l)\mathcal{F}_l\big)' - \sum_{k\in S} c_{pk} T' \mathcal{F}_k - \sum_{k\in S} h_k m_k \omega_k. \tag{2.34}$$

It is worthwhile to point out several differences between the temperature equation (2.34) and the temperature equations considered in previous work. In all previous work, it has been assumed that the species specific heats are species independent, that is, $c_{pk} = \overline{c}_p$, $k \in S$. In this situation, one has

$$\sum_{k\in S} c_{pk} T' \mathcal{F}_k = \overline{c}_p\, T' \left(\sum_{k\in S} \mathcal{F}_k\right) = 0,$$

anticipating the mass constraint $\sum_{k\in S} \mathcal{F}_k = 0$. In this situation, one also has

$$\sum_{k\in S} h_k m_k \omega_k = \sum_{k\in S} h_k^0 m_k \omega_k,$$

anticipating the mass conservation relation $\sum_{k\in S} m_k \omega_k = 0$, since the temperature dependent part of the enthalpies $k_k - h_k^0 = \overline{c}_p(T - T^0)$ are identical. Moreover, the transport and specific heats coefficients were generally assumed to be constant with a resulting simplified equation in the form

$$c\,\overline{c}_p T' = \lambda T'' - \sum_{k\in S} h_k^0 m_k \omega_k.$$

In comparison, we first note that in (2.34) the source term $\sum_{k\in S} h_k m_k \omega_k$ is not bounded a priori even when assuming that the rate ω_k, $k \in S$, are bounded, since the enthalpies are linearly increasing functions of temperature. In addition there is a quadratic derivative term $\sum_{k\in S} c_{pk} T' \mathcal{F}_k$, and the coefficients λ and c_p are not constants. Finally, maximum principles cannot be used when thermal diffusion is included, that is, when $\widetilde{\chi}$ is nonzero.

2.7. Boundary conditions

We now specify the flame boundary conditions at the cold and hot boundaries. We assume that the cold boundary is on the left side and the hot equilibrium boundary on the right side.

The right boundary conditions is in the form

$$\xi(\infty) = \xi^{\mathrm{e}} \qquad (2.35),$$

where ξ^{e} is an equilibrium point where the source term vanish $w(\xi^{\mathrm{e}}) = 0$. Existence and uniqueness of the proper equilibrium ξ^{e} is established in Section 3. In particular, this equilibrium state is such that $Y^{\mathrm{e}} > 0$, that is, satisfies $Y_k^{\mathrm{e}} > 0$, $k \in S$, where the superscript $^{\mathrm{e}}$ is used to denote the value at $\xi = \xi^{\mathrm{e}}$ of any function of the state variables.

On the other hand, we consider two types of cold boundary conditions. The first type corresponds to the anchored flame model with an unknown function ξ defined on the the half line $[0, \infty)$ and with the boundary conditions

$$c(\xi(0) - \xi^{\mathrm{f}}) + \phi(0) = 0, \qquad (2.36)$$

and

$$T(0) = T^{\mathrm{i}}, \qquad (2.37)$$

where ξ^{f} is a given nonequilibrium state and T^{i} is a temperature such that $T^{\mathrm{f}} < T^{\mathrm{i}}$. The state ξ^{f} is such that $Y^{\mathrm{f}} \geq 0$, $\sum_{k \in S} Y_k^{\mathrm{f}} = 1$, and such that each species of the mixture is reachable from Y^{f} by the chemical network. The superscript $^{\mathrm{f}}$ is used to denote the value at $\xi = \xi^{\mathrm{f}}$ of any function of the state variables.

The anchored flame model has been introduced by Hirschfelder, Curtiss and Campbell [HCC53]. This model corresponds to an idealized adiabatic flame holder located at the origin. The anchored flame model supresses the cold boundary difficulty without any artificial modification of the source term [HCC53] [BL82] [Wil85]. This model also corresponds to practical experimental configurations. Indeed, it is possible to inject a reactive mixture through a porous plate in a tube and to stabilize a flame far from the injection device by using laser tomography which triggers the injection velocity [Q*al*84] [Cla85]. For such flames, by integrating the conservation equations through the adiabatic porous burner, we obtain Equation (2.36). By choosing a temperature T^{i} slightly above the cold mixture temperature, we then recover the model. For exothermic systems, the temperature T^{i} can also be interpreted as an ignition temperature [Wil85]. Finally, the boundary conditions (2.36) (2.37) are also used in numerical modeling of complex chemistry flames [Ser86] [GS92].

It is also possible to consider an unknown function ξ is defined on the real line $(-\infty, \infty)$ and to replace (2.36) by the condition

$$\xi(-\infty) = \xi^{\mathrm{f}}. \qquad (2.38)$$

The relation (2.37) is still needed in order to remove the translational invariance of the model. However, it is well known that the chemistry source terms only vanish at equilibrium points, so that we have $w(\xi^{\mathrm{f}}) \neq 0$ and (2.38) cannot be satisfied. This problem is the well known "cold boundary difficulty". Various cutoff functions ψ have then been used to modify the source terms w into ψw, in order to satisfy the boundary condition (2.38). In this paper, we consider a cutoff function in the form $\psi(x) = 1_{[0,\infty)}(x)$ and thus source terms in the form $1_{[0,\infty)}w$. For this cutoff function, we establish rigorously in Section 5 that both formulations on $(-\infty,\infty)$ and $[0,\infty)$ are equivalent. As a consequence, it will be sufficient to investigate the anchored flame problem on $[0,\infty)$.

Note that when a continuous function of the state variables is used as a cutoff function, it introduces artificial equilibrium points in the phase space, and the dynamics of the reactive system has to guarantee that such artificial points are not further reached in the flame. For a priori exothermic systems, any increasing function of temperature can be used as a cutoff function. However, this is no longer the case for arbitrary reversible chemical networks, due to the lack of a priori monotonicity of the temperature and more generally of state functions when multicomponent transport is considered.

Remark 2.4. A model with a cutoff term ψ which is a continuous function of temperature has been used by A. Bonnet in [Bon92] [Bon94]. The flame model considered in this paper corresponds to a generalized chemistry of irreversible type and to the simple transport model $\phi = -d\,\xi'$ where d is a constant. However, it turns out that Bonnet's proof that the flame does not reach again the ignition temperature T^{i} is wrong.

Indeed, Bonnet has used strong solutions of (2.1) with a modified source term $1_{[T^{\mathrm{a}},\infty)}(T)\ w$ involving a temperature dependent Heavyside function $1_{[T^a,\infty)}(T)$ with $T^{\mathrm{a}} = T^{\mathrm{i}} + \epsilon$. Bonnet is claiming the existence of solutions of the modified equations whose second derivatives are Lipchitz continuous and which satisfy *pointwise* the modified governing equations. He then shows that these solutions are indeed solutions of the original equation since one establishes that $T \geq T^{\mathrm{a}}$ when the source term is $1_{[T^{\mathrm{a}},\infty)}(T)\ w$. This yields a lower bound for the temperature of the original problem with a non modified source term. However, these strong solutions do not exist. Indeed, the existence argument of Bonnet is first wrong since when $\psi_k(z) \to 1_{[T^{\mathrm{a}},\infty)}(z)$ pointwise as $k \to \infty$, where ψ_k is continuous, and when $T_k \to T$ by a compacity argument, then we do *not* have $\psi_k(T_k) \to 1_{[T^{\mathrm{a}},\infty)}(T)$ pointwise since $z \to 1_{[T^{\mathrm{a}},\infty)}(z)$ is discontinuous. Moreover, one can easily build the counterexemple $-du'' = 1$ over $[-2,2]$ with $u(-2) = 2$ and $u(2) = 2$ whose solution is $u(x) = x^2/2$. If a solution "à la Bonnet" of $-dv'' = 1_{v\geq 1}$ would exist, one would get $v \geq 1$ and thus $u = v$, which is absurd. ∎

Remark 2.5. Note the difference between anchored flames and burner stabilized flames for which the mass flux is imposed. Denoting by c^{f} this prescribed mass flux, burner stabilized flames satisfy the boundary conditions

$$c^{\mathrm{f}}\big(Y(0) - Y^{\mathrm{f}}\big) + \mathcal{F}(0) = 0. \tag{2.39}$$

$$T(0) = T^{\mathrm{f}}, \tag{2.40}$$

and the imposed mass flux c^{f} is such that $0 < c^{\mathrm{f}} < c$ where c is the eigenvalue of the anchored flame problem. The anchored flame problem thus corresponds to the idealized limit of an adiabatic burner with $c\big(h(0) - h^{\mathrm{f}}\big) + q(0) = 0$, whereas heat losses are present for burner stabilized flames with $T(0) = T^{\mathrm{f}}$. ∎

3. THERMOCHEMISTRY AND EQUILIBRIUM POINTS

In this section we specify the mathematical assumptions concerning the thermodynamic functions and the source terms. We then characterize the equilibrium state ξ^{e} as a unique equilibrium point in a given conservation manifold. From this characterization, we establish existence and uniqueness of the equilibrium state ξ^{e}. We also investigate various thermodynamic functions over element conservation manifolds for future a priori estimates.

3.1. Thermodynamics

The mathematical assumptions concerning thermodynamic properties are the following.

(H_1) The species molar masses m_k, $k \in S$, and the gas constant R are positive constants. The formations enthalpies h_k^0, $k \in S$, and the formation entropies s_k^{0p}, $k \in S$, are constants. The specific heats c_{pk}, $k \in S$, are C^∞ functions of $T \in [0, \infty)$. Furthermore, there exist positive constants $\underline{c}_p$ and $\overline{c}_p$ with $0 < \underline{c}_p \leq c_{pk}(t) \leq \overline{c}_p$, for $t \geq 0$, and $k \in S$.

Note that the thermodynamic functions c_{pk}, $k \in S$, and h_k, $k \in S$, are defined for $T \geq 0$, so that c_p and h are defined for $T \geq 0$ and $Y \geq 0$. On the other hand, the functions s_k, $k \in S$, g_k, $k \in S$, and μ_k, $k \in S$, and s, are only defined for $T > 0$ and $Y > 0$. One may also easily check that the domain of definition of s can be extented to $T > 0$ and $Y \geq 0$, $Y \neq 0$ by using $0 \log 0 = 0$. Nevertheless, the gas species specific heats, and thus the enthalpies, are defined up to zero temperature, but not the gas entropy which explodes like $\log T$. The extension up to zero temperature of specific heats and enthalpies is commonly used in thermodynamics. However, the entropy is unbounded for small temperatures since we consider gaseous mixtures.

From assumption (H_1) we first obtain that the various thermodynamic functions are smooth. Since the pressure p is constant, all thermodynamic properties have also been defined in terms of (T, Y). Since the natural conserved variables in flame problems are (h, Y), we now investigate the map $\Xi : (T, Y) \to (h, Y)$.

Lemma 3.1. *The map $\Xi : (T, Y) \to (h, Y)$ is a C^∞ diffeomorphism from $T > 0$, $Y \geq 0$, $Y \neq 0$, onto $\mathcal{H}$ where*

$$\mathcal{H} = \{\ (h, Y),\ h > \sum_{k \in S} Y_k h_k(0),\ Y \geq 0,\ Y \neq 0\ \}. \tag{3.1}$$

Proof. This comes directly from the formula

$$h(T, Y) = \sum_{k \in S} Y_k h_k(0) + \int_0^T \Big(\sum_{k \in S} Y_k c_{pk}(t) \Big)\, dt,$$

and the positivity properties of the specific heats c_{pk}, $k \in S$. ■

Lemma 3.2. *Denote by σ the function defined over $\mathcal{H}$ by*

$$\sigma(h,Y) = s\big(\Xi(h,Y)\big) = s(T,Y). \tag{3.2}$$

Then we have

$$\partial_h \sigma = \partial_{\xi_0}\sigma = \frac{1}{T}, \qquad \partial_{Y_k}\sigma = \partial_{\xi_k}\sigma = -\frac{g_k}{T} = -R\,\mu_k, \quad k \in S, \tag{3.3}$$

and the Euler relation $\sigma = \langle \partial_\xi \sigma, \xi\rangle$ holds. Furthermore, $\partial_\xi^2\sigma$ is given by

$$-\frac{\big\langle(\partial^2_{\xi_k\xi_l}\sigma)x,x\big\rangle}{R} = \frac{(x_0 - \sum_{k\in S} h_k x_k)^2}{RT^2 c_p} + \sum_{k\in S}\frac{(x_k/m_k)^2}{Y_k/m_k} - \frac{(\sum_{k\in S} x_k/m_k)^2}{\sum_{l\in S} Y_l/m_l}, \tag{3.4}$$

where $\langle x,y\rangle$ denotes the scalar product between vectors x and y. As a consequence, σ is concave and $N(\partial_\xi^2\sigma) = \mathbb{R}\xi$.

The proof of Lemma 3.2 is straightforward and is omitted. In order to simplify the notation, we will most of the time use a single symbol in order to denote a function of (T,Y) or a function of (h,Y) with an exception for σ. We will further need the matrix A defined by $A = d_Y X$ and a direct calculation yields

$$\begin{cases} A_{kk} = \dfrac{\overline{m}}{m_k} + \gamma_k\Big(1 - \dfrac{\overline{m}}{m_k}\Big), & k \in S, \\ A_{kl} = \gamma_k\Big(1 - \dfrac{\overline{m}}{m_l}\Big), & k,l \in S, \quad k \neq l. \end{cases} \tag{3.5}$$

It is interesting to note that the matrix $A = d_Y X$ is invertible and that we have $AY = X$ where $X = (X_1,\dots,X_n)^\star$ [Gio90].

3.2. Thermochemistry

We introduce here a set of assumptions concerning the chemical reactions and the chemical production rates. The reactive species are assumed to be constituted by elements and we denote by $\mathcal{E}_{kl}$ the number of l^{th} element in the k^{th} species. We also denote by $E = [1, n_E]$ the set of element indices and by $n_E \geq 1$ the number of elements.

(H_2) The stoichiometric coefficients ν^{d}_{ki}, and ν^{r}_{ki}, $k \in S$, $i \in R$, and the element coefficients $\mathcal{E}_{kl}$, $k \in S$, $l \in E$, are nonnegative integers. The element vectors $\mathcal{E}_l$, $l \in E$, defined by $\mathcal{E}_l = (\mathcal{E}_{1l},\dots,\mathcal{E}_{nl})^\star$, and the reaction vectors ν_i, $i \in R$, defined by $\nu_i = (\nu_{1i},\dots,\nu_{ni})^\star$, satisfy the element conservation relations

$$\langle \nu_i, \mathcal{E}_l\rangle = 0, \qquad i \in R, \quad l \in E. \tag{3.6}$$

We also define the vectors $\nu^{\mathrm{d}}_i = (\nu^{\mathrm{d}}_{1i},\dots,\nu^{\mathrm{d}}_{ni})^\star$, and $\nu^{\mathrm{r}}_i = (\nu^{\mathrm{r}}_{1i},\dots,\nu^{\mathrm{r}}_{ni})^\star$, $i \in R$, which satisfy $\langle \nu^{\mathrm{d}}_i, \mathcal{E}_l\rangle = \langle \nu^{\mathrm{r}}_i, \mathcal{E}_l\rangle$, $i \in R$. The space spanned by the reaction vectors is denoted by $\mathcal{R} = \mathrm{span}\{\ \nu_i,\ i \in R\ \}$ and the space spanned by the element vectors is denoted by $\mathcal{E} = \mathrm{span}\{\ \mathcal{E}_l,\ l \in E\ \}$ in such a way that $\mathcal{R} \subset \mathcal{E}^\perp$ and $\mathcal{E} \subset \mathcal{R}^\perp$.

(H_3) The element masses $\widetilde{m}_l$, $l \in E$, are positive constants and the species molar masses m_k, $k \in S$, are given by

$$m_k = \sum_{l \in E} \widetilde{m}_l \, \mathcal{E}_{kl}. \tag{3.7}$$

Denoting by m the mass vector $m = (m_1, \dots, m_n)^\star$, these relations can be written in vector form

$$m = \sum_{l \in E} \widetilde{m}_l \, \mathcal{E}_l. \tag{3.8}$$

Remark 3.3. The elements may taken to be the atomic elements provided that the corresponding vectors are independent. When this is not the case, it is first necessary to eliminate linearly dependent atomic elements. For realistic complex chemistry networks, the number of chemical reactions is always much larger than the number of chemical species and one usually has $\mathcal{R} = \mathcal{E}^\perp$. In other words, the chemical reactions are spanning the largest possible space. When this is not the case, one has simply to use the space $\mathcal{R}^\perp$ instead of $\mathcal{E}$ [Kra70]. ∎

In the following, we also have to use the mass weighted production rates $m_k\omega_k$, $k \in S$. To this purpose, we introduce the mass weights matrix M, of order n, defined by

$$M = \mathrm{diag}(m_1, \dots, m_n). \tag{3.9}$$

The mass weighted stoichiometric coefficients are then the vectors $M\nu_i$, $i \in R$, and the specific element compositions are the vectors $M^{-1}\mathcal{E}_l$, $l \in E$. The corresponding spaces $M\mathcal{R}$ and $M^{-1}\mathcal{E}$, spanned by these mass weighted vectors, are then such that $M\mathcal{R} \subset (M^{-1}\mathcal{E})^\perp$ and $M^{-1}\mathcal{E} \subset (M\mathcal{R})^\perp$ in the composition phase space $\mathbb{R}^n$. From element conservation and the definition of species masses, we first deduce the following mass conservation properties.

Lemma 3.4. *The vector of chemical production rates $\omega = (\omega_1, \dots, \omega_n)^\star$ can be written in vector form*

$$\omega = \sum_{i \in R} r_i \, \nu_i, \tag{3.10}$$

so that $\omega \in \mathcal{R}$ and $M\omega \in M\mathcal{R}$. In addition, the unity vector $U \in \mathbb{R}^n$ defined by $U = (1, \dots, 1)^\star$, satisfies $U \in (M\mathcal{R})^\perp$ so that we have the total mass conservation relation

$$\langle U, M\omega \rangle = \sum_{k \in S} m_k \omega_k = 0. \tag{3.11}$$

Proof. These properties are straightforward from (H_2) and (H_3) which imply that

$$U = \sum_{l \in E} \widetilde{m}_l M^{-1} \mathcal{E}_l, \tag{3.12}$$

so that $U \in (M\mathcal{R})^\perp$. ∎

3.3. Alternate expressions for the chemical production rates

It will be usefull in the following to decompose the production rates between the creation and destruction rates.

Lemma 3.5. *The chemical production rates ω_k, $k \in S$, can be split into*

$$\omega_k = \mathcal{P}_k - Y_k \widehat{\mathcal{N}}_k, \qquad k \in S, \tag{3.13}$$

where $\mathcal{P}_k$ and $\widehat{\mathcal{N}}_k$, are respectively the creation and reduced destruction rates of the k^{th} species. These rates are such that $\mathcal{P}_k \geq 0$, $\widehat{\mathcal{N}}_k \geq 0$, and are smooth functions of (T, Y), for $T > 0$, $Y \geq 0$, $Y \neq 0$.

Proof. We simply use (2.22)–(2.24) and write that $\omega_k = \mathcal{P}_k - \mathcal{N}_k$, where

$$\mathcal{P}_k = \sum_{i \in R} \Big(\nu_{ki}^{\mathrm{r}} K_i^{\mathrm{d}} \prod_{l \in S} \gamma_l^{\nu_{li}^{\mathrm{d}}} + \nu_{ki}^{\mathrm{d}} K_i^{\mathrm{r}} \prod_{l \in S} \gamma_l^{\nu_{li}^{\mathrm{r}}} \Big), \tag{3.14}$$

and

$$\mathcal{N}_k = \sum_{i \in R} \Big(\nu_{ki}^{\mathrm{d}} K_i^{\mathrm{d}} \prod_{l \in S} \gamma_l^{\nu_{li}^{\mathrm{d}}} + \nu_{ki}^{\mathrm{r}} K_i^{\mathrm{r}} \prod_{l \in S} \gamma_l^{\nu_{li}^{\mathrm{r}}} \Big). \tag{3.15}$$

Since the stoichiometric coefficients are nonnegative integers, we can now write that

$$\mathcal{N}_k = \gamma_k \Big(\sum_{\substack{i \in R \\ \nu_{ki}^{\mathrm{d}} \geq 1}} \nu_{ki}^{\mathrm{d}} K_i^{\mathrm{d}} \gamma_k^{\nu_{ki}^{\mathrm{d}} - 1} \prod_{\substack{l \in S \\ l \neq k}} \gamma_l^{\nu_{li}^{\mathrm{d}}} + \sum_{\substack{i \in R \\ \nu_{ki}^{\mathrm{r}} \geq 1}} \nu_{ki}^{\mathrm{r}} K_i^{\mathrm{r}} \gamma_k^{\nu_{ki}^{\mathrm{r}} - 1} \prod_{\substack{l \in S \\ l \neq k}} \gamma_l^{\nu_{li}^{\mathrm{r}}} \Big), \tag{3.16}$$

so that $\mathcal{N}_k = Y_k \widehat{\mathcal{N}}_k$, $k \in S$, where

$$\widehat{\mathcal{N}}_k = \frac{1}{m_k} \Big(\sum_{l \in S} \frac{Y_l}{m_l} \Big)^{-1} \Big(\sum_{\substack{i \in R \\ \nu_{ki}^{\mathrm{d}} \geq 1}} \nu_{ki}^{\mathrm{d}} K_i^{\mathrm{d}} \gamma_k^{\nu_{ki}^{\mathrm{d}} - 1} \prod_{\substack{l \in S \\ l \neq k}} \gamma_l^{\nu_{li}^{\mathrm{d}}} + \sum_{\substack{i \in R \\ \nu_{ki}^{\mathrm{r}} \geq 1}} \nu_{ki}^{\mathrm{r}} K_i^{\mathrm{r}} \gamma_k^{\nu_{ki}^{\mathrm{r}} - 1} \prod_{\substack{l \in S \\ l \neq k}} \gamma_l^{\nu_{li}^{\mathrm{r}}} \Big), \tag{3.17}$$

which is a smooth function of (T, Y), for $T > 0$, $Y \geq 0$, $Y \neq 0$. ■

We now rewrite the rate of progress (2.24) by introducing new reaction constants, making use of the equilibrium constants. We define $\widehat{K}_i$, $i \in R$, by

$$\log \widehat{K}_i = \log K_i^{\mathrm{d}}(T) - \langle M\nu_i^{\mathrm{d}}, \mu^p \rangle = \log K_i^{\mathrm{r}}(T) - \langle M\nu_i^{\mathrm{r}}, \mu^p \rangle, \tag{3.18}$$

where $\mu_k^p = g_k^p/(RT)$, $k \in S$, using $\log K_i^{\mathrm{e}} = -\langle M\nu_i, \mu^p \rangle = \langle M\nu_i^{\mathrm{d}}, \mu^p \rangle - \langle M\nu_i^{\mathrm{r}}, \mu^p \rangle$, for $i \in R$. We can then rewrite (2.24) in the form

$$r_i = \widehat{K}_i \Big(\exp\langle M\nu_i^{\mathrm{d}}, \mu^p \rangle \prod_{k \in S} \gamma_k^{\nu_{ki}^{\mathrm{d}}} - \exp\langle M\nu_i^{\mathrm{r}}, \mu^p \rangle \prod_{k \in S} \gamma_k^{\nu_{ki}^{\mathrm{r}}} \Big), \tag{3.19}$$

and from the definition $\mu_k = \mu_k^p + (1/m_k) \log \gamma_k$, $k \in S$, we finally obtain that

$$r_i = \widehat{K}_i \Big(\exp\langle M\nu_i^{\mathrm{d}}, \mu \rangle - \exp\langle M\nu_i^{\mathrm{r}}, \mu \rangle \Big). \tag{3.20}$$

The assumptions concerning the rate constants can then be written in terms of the quantities $\widehat{K}_i$, $i \in R$.

(H_4) The rate constants $\widehat{K}_i$, $i \in R$, are C^∞ positive functions of $T \in (0, \infty)$.

Note that we neither assume that the quantities K_i^{d}, $i \in R$, or K_i^{r}, $i \in R$, are bounded functions of the temperature T, as in previous studies, nor that the quantities $\widehat{K}_i$, $i \in R$, are bounded.

3.4. Equilibrium points

In this section, we first restate that detailed balance holds at any equilibrium point. We then establish existence and uniqueness of the proper equilibrium point.

Proposition 3.6. *The reduced entropy production due to chemical reactions*

$$\zeta(T, Y) = -\langle \mu, M\omega \rangle = -\frac{1}{RT} \sum_{k \in S} g_k m_k \omega_k,$$

defined for $T > 0$ and $Y > 0$, is nonnegative and admits 0 as a minimum at any point where source terms vanish. Any point $(T^{\mathrm{e}}, Y_1^{\mathrm{e}}, \dots, Y_n^{\mathrm{e}})$ with $T^{\mathrm{e}} > 0$ and $Y_k^{\mathrm{e}} > 0$, $k \in S$, where the source term vanishes

$$\omega_k(T^{\mathrm{e}}, Y_1^{\mathrm{e}}, \dots, Y_n^{\mathrm{e}}) = 0, \qquad k \in S, \tag{3.21}$$

is also such that the rates of progress of each reaction vanish

$$r_i(T^{\mathrm{e}}, Y_1^{\mathrm{e}}, \dots, Y_n^{\mathrm{e}}) = 0, \qquad i \in R, \tag{3.22}$$

which can also be written in the form

$$\Big\langle \mu(T^{\mathrm{e}}, Y_1^{\mathrm{e}}, \dots, Y_n^{\mathrm{e}}), M\nu_i \Big\rangle = 0, \qquad i \in R. \tag{3.23}$$

Proof. Rewritting ζ in the form

$$\zeta = -\frac{1}{RT} \sum_{\substack{i \in R \\ k \in S}} g_k m_k \nu_{ki} r_i = -\sum_{i \in R} \big\langle \mu, M(\nu_i^{\mathrm{r}} - \nu_i^{\mathrm{d}}) \big\rangle \, r_i,$$

and using (3.20), we obtain that

$$\zeta = \sum_{i \in R} \widehat{K}_i \Big(\langle \mu, M\nu_i^{\mathrm{d}} \rangle - \langle \mu, M\nu_i^{\mathrm{r}} \rangle \Big) \Big(\exp\langle \mu, M\nu_i^{\mathrm{d}} \rangle - \exp\langle \mu, M\nu_i^{\mathrm{r}} \rangle \Big), \tag{3.24}$$

so that $\zeta(T, Y) \geq 0$ and $\zeta(T, Y) = 0$ if and only if $\langle \mu, M\nu_i \rangle = 0$, $i \in R$, that is to say, if and only if $r_i = 0$, $i \in R$. In addition, $r_i = 0$, $i \in R$, if and only if $\omega_k = 0$, $k \in S$, from the expression of ζ. ∎

Definition 3.7. *A point $(T^{\mathrm{e}}, Y_1^{\mathrm{e}}, \dots, Y_n^{\mathrm{e}})$ with $T^{\mathrm{e}} > 0$ and $Y^{\mathrm{e}} > 0$ which satisfies the equivalent properties of Proposition 3.6 will be termed an equilibrium point.*

In order to characterize the equilibrium point ξ^{e}, we now multiply (2.1) by any vector $u \in (M\mathcal{R})^{\perp}$ and we obtain that

$$c\,\langle Y, u\rangle' + \langle \mathcal{F}, u\rangle'' = 0. \tag{3.25),}$$

Integrating formally over $[0, \infty)$—or equivalently over $(-\infty, \infty)$—we deduce that

$$\langle Y^{\mathrm{e}} - Y^{\mathrm{f}}, u\rangle = 0, \tag{3.26}$$

keeping in mind that we only seek solutions with a positive mass flow rate c. Note that such formal integrations can easily be rigorously justified. As a consequence, the equilibrium point ξ^{e} must be such that $Y^{\mathrm{e}} \in Y^{\mathrm{f}} + M\mathcal{R}$. Similarly, integrating (2.2) yields that

$$h^{\mathrm{e}} = h^{\mathrm{f}}, \tag{3.27}$$

and from the isobaric approximation we also have $p^{\mathrm{e}} = p^{\mathrm{f}} = p$.

As a consequence, we have to investigate existence and uniqueness of the equilibrium point in the affine submanifold $Y^{\mathrm{f}} + M\mathcal{R}$ with a given specific enthapy $h^{\mathrm{e}} = h^{\mathrm{f}}$. Existence of equilibrium states is generally obtained by extremalizing a functional over a conservation manifold. The functional to be maximized or minimized depends on which thermal properties are kept fixed [SS65] [Kra70]. In our situation, since we impose the pressure p and the specific enthalpy h, the proper functional to be maximized is the specific entropy σ. Moreover, there are two variants depending if the formulation is in terms of constrained [SS65] or free [Kra70] variables. The former method is more suited to the mas fractions variables and will be used in this paper.

From the above consideration, we seek for the equilibrium mass fractions Y^{e} in the conservation simplex

$$\mathcal{X} = (Y^{\mathrm{f}} + M\mathcal{R}) \cap (0, \infty)^n \cap \{\, Y, \sum_{k \in S} Y_k h_k(0) < h^{\mathrm{f}} \,\}. \tag{3.28}$$

In order to establish existence and uniqueness of the equilibrium ξ^{e}, we assume that $T^{\mathrm{f}} > 0$, $Y^{\mathrm{f}} \geq 0$, $\langle Y^{\mathrm{f}}, U\rangle = 1$ and that $(Y^{\mathrm{f}} + M\mathcal{R}) \cap (0, \infty)^n \neq \emptyset$. When the latter property does not hold, we simply have to eliminate species from the network. This property is weaker than the reachability property needed for homogeneous reactors introduced in [VH85].

Proposition 3.8. *Assume that (H_1)–(H_4) hold, that $\xi^{\mathrm{f}} \in \mathcal{H}$, $Y^{\mathrm{f}} \geq 0$, $\langle Y^{\mathrm{f}}, U\rangle = 1$, $(Y^{\mathrm{f}} + M\mathcal{R}) \cap (0, \infty)^n \neq \emptyset$. Then there exists a unique equilibrium vector Y^{e} in the simplex $\mathcal{X}$ where the source term ω vanishes. At Y^{e}, the reaction rates of progress also vanish and $\mu^{\mathrm{e}} \in (M\mathcal{R})^{\perp}$.*

Proof. First note that $\mathcal{X}$ is nonempty since there exists $Y^{\mathrm{p}} \in Y^{\mathrm{f}} + M\mathcal{R}$ with $Y^{\mathrm{p}} > 0$ so that $(1-\tau)Y^{\mathrm{f}} + \tau Y^{\mathrm{p}}$ is in $\mathcal{X}$ for small positive τ. We characterize the equilibrium point Y^{e} as the only extremum of the function $Y \to \sigma(h^{\mathrm{f}}, Y)$ which is a C^{∞} function of Y over $\mathcal{X}$. The partial derivative of $\sigma(h^{\mathrm{f}}, Y)$ with respect to the mass fractions Y is

$$\partial_Y \sigma(h^{\mathrm{f}}, Y) = -R\mu,$$

and $\sigma(h^{\mathrm{f}},Y)$ is strictly concave over the convex set $\mathcal{X}$. Indeed, we have from (3.4)

$$-\frac{1}{R}\sum_{k,l\in S}\big(\partial^2_{Y_kY_l}\sigma(h^{\mathrm{f}},Y)\big)x_kx_l=\sum_{k\in S}\frac{(x_k/m_k)^2}{Y_k/m_k}-\frac{\left(\sum_{k\in S}x_k/m_k\right)^2}{\sum_{l\in S}Y_l/m_l},\tag{3.29}$$

so that $\partial^2_Y\sigma(h^{\mathrm{f}},Y)$ is negative semidefinite and $N\big(\partial^2_Y\sigma(h^{\mathrm{f}},Y)\big)=\mathbb{R}Y$. However, we have $Y\notin M\mathcal{R}$ from $M\mathcal{R}\subset U^\perp$ and $Y\notin U^\perp$ since $Y>0$ over $\mathcal{X}$.

Because we want to maximize $\sigma(h^{\mathrm{f}},Y)$, we only need to consider the subset $\mathfrak{X}$

$$\mathfrak{X}=\{\,Y\in\mathcal{X},\ \sigma(h^{\mathrm{f}},Y)>\sigma(\xi^{\mathrm{f}})-1\,\}.$$

This set $\mathfrak{X}$ is convex since σ is concave, is nonempty since $(1-\tau)Y^{\mathrm{f}}+\tau Y^{\mathrm{p}}\in\mathfrak{X}$ for τ small and positive. The mass fractions are bounded over $\mathfrak{X}$ since $Y\in\mathfrak{X}$ implies $Y>0$ and $\langle Y,U\rangle=\langle Y^{\mathrm{f}},U\rangle$ from the mass conservation constraint $U\in(M\mathcal{R})^\perp$. Moreover, over the set $\mathfrak{X}$, the temperature $T(h^{\mathrm{f}},Y)$ is easily seen to be positively bounded from below since σ is bounded from below. This implies that there exists a positive α

$$\Xi^{-1}\big(\mathfrak{X}\big)\ \subset\ \{\ (T,Y);\ \alpha\le T,\ Y\ge0,\ \langle Y,U\rangle=1\ \},$$

where s is defined and continuous. As a consequence, the function $\sigma(h^{\mathrm{f}},Y)$ can be extended over the closure $\overline{\mathfrak{X}}$ of $\mathfrak{X}$. Therefore, $\sigma(h^{\mathrm{f}},Y)$ admits a maximum on this convex compact set. Denoting Y^{m} any point where the maximum is reached, we claim that Y^{m} is not on the boundary of $\mathfrak{X}$. Of course, it cannot be reached at the boundary $\sigma=\sigma(\xi^{\mathrm{f}})-1$. On the other hand, it can neither be reached at the boundaries $Y_k=0$, $k\in S$. Indeed, considering any point Y^{in} in the interior of $\mathfrak{X}$, the function $u(\tau)=\sigma\big(h^{\mathrm{f}},\tau Y^{\mathrm{in}}+(1-\tau)Y^{\mathrm{m}}\big)$ is continuous over $[0,1]$, differentiable over $(0,1]$ and reaches its maximum for $\tau=0$. However, over the interval $(0,1]$, the derivative of u is given by

$$u'(t)=\langle\partial_Y\sigma,Y^{\mathrm{in}}-Y^{\mathrm{m}}\rangle=-\sum_{\substack{k\in S\\ Y_k^{\mathrm{m}}=0}}(\partial_{Y_k}\sigma)Y_k^{\mathrm{in}}+\sum_{\substack{k\in S\\ Y_k^{\mathrm{m}}>0}}(\partial_{Y_k}\sigma)(Y_k^{\mathrm{in}}-Y_k^{\mathrm{m}}),$$

with $\partial_Y\sigma$ evaluated at $\big(h^{\mathrm{f}},\tau Y^{\mathrm{in}}+(1-\tau)Y^{\mathrm{m}}\big)$. This implies that u' is positive in the neighborhood of $\tau=0$, since $\partial_{Y_k}\sigma\big(h^{\mathrm{f}},\tau Y^{\mathrm{in}}+(1-\tau)Y^{\mathrm{m}}\big)$ goes to $-\infty$ for $\tau\to0$ when $Y_k^{\mathrm{m}}=0$ whereas the sum over $Y_k^{\mathrm{m}}>0$ remains bounded, an obvious contradiction. As a consequence, $\sigma(h^{\mathrm{f}},Y)$ reaches its maximum in the interior of $\mathcal{X}$, and, thanks to the strict concavity of $\sigma(h^{\mathrm{f}},Y)$, this maximum is unique and we denote by Y^{e} the corresponding point.

Since this maximum is reached in the interior of $\mathfrak{X}$ we must have

$$\mu^{\mathrm{e}}=\mu(h^{\mathrm{e}},Y^{\mathrm{e}})\in(M\mathcal{R})^\perp.\tag{3.30}$$

As a consequence, $\zeta=-\langle\mu,M\omega\rangle$ vanishes at $(h^{\mathrm{e}},Y^{\mathrm{e}})$ which is therefore an equilibrium point. Conversely, from Proposition 3.7, any equilibrium point on the simplex $\mathcal{X}$ is such that the quantities $\langle\mu,M\nu_i\rangle$, $i\in R$, vanish so that the partial derivatives of $\sigma(h^{\mathrm{f}},Y)$ along the simplex are zero. Since $\sigma(h^{\mathrm{f}},Y)$ is a strictly concave function over

$\mathcal{X}$, it reaches a maximum at this point. Therefore, this point coincides with the unique maximum of $\sigma(h^{\mathrm{f}}, Y)$ and the proof is complete. ∎

In the following proposition, we investigate how the equilibrium point ξ^{e} depends on the cold state ξ^{f} following [Kra70].

Proposition 3.9. *Denote by Q the orthogonal projector onto $(0, M\mathcal{R})^{\perp}$. Then the equilibrium point ξ^{e} only depends on $Q(\xi^{\mathrm{f}})$ and is a smooth function of $Q(\xi^{\mathrm{f}})$.*

Proof. The equilibrium point ξ^{e} only depends on $Q(\xi^{\mathrm{f}})$ by construction. Denote by $v_1, \ldots, v_n$ an orthonormal basis of $\mathbb{R}^n$ such that $v_1, \ldots, v_d$ is a basis of $M\mathcal{R}$ and $v_{d+1}, \ldots, v_n$ a basis of $(M\mathcal{R})^{\perp}$, where $d = \dim(\mathcal{R})$. The vectors $(1, O)^{\star}$—where $O = (0, \ldots, 0)^{\star} \in \mathbb{R}^n$—and $(0, v_i)^{\star}$, for $d+1 \leq i \leq n$, form a basis of $(0, M\mathcal{R})^{\perp}$ and the corresponding components of $Q(\xi^{\mathrm{f}})$ are $h^{\mathrm{f}} = \langle \xi^{\mathrm{f}}, (1, O)^{\star} \rangle$ and $\langle Y^{\mathrm{f}}, v_i \rangle$, $d+1 \leq i \leq n$, respectively. The equilibrium point ξ^{e} is then the unique solution (h, Y) of the system

$$\begin{cases} \qquad\qquad h = h^{\mathrm{f}}, & \\ \quad \langle Y, v_i \rangle = \langle Y^{\mathrm{f}}, v_i \rangle, & d+1 \leq i \leq n, \\ \langle \mu(h, Y), v_i \rangle = 0, & 1 \leq i \leq d. \end{cases}$$

The jacobian matrix of this system is easily shown to have full rank at equilibrium ξ^{e} since $N(\partial_Y \mu) \cap (M\mathcal{R}) = \{0\}$, so that the implicit function theorem applies. ∎

Finally, the assumptions concerning the cold state ξ^{f} and the equilibrium temperature T^{e} are the following.

(H_5) The cold state ξ^{f} is such that $\xi^{\mathrm{f}} \in \mathcal{H}$, so that $T^{\mathrm{f}} > 0$ and $Y^{\mathrm{f}} \geq 0$. The mass fractions Y^{f} also satisfy $\langle Y^{\mathrm{f}}, U \rangle = 1$ and

$$(Y^{\mathrm{f}} + M\mathcal{R}) \cap (0, \infty)^n \neq \emptyset,$$

and we have $T^{\mathrm{f}} < T^{\mathrm{i}} < T^{\mathrm{e}}$.

3.5. A local stability inequality

In this section we restate a stability inequality first derived by Boillat and Pousin under similar assumptions [Boi95] [Pou93]. Remark first that the manifold $\xi^{\mathrm{f}} + (0, M\mathcal{R})$ can also be written $Q(\xi) = Q(\xi^{\mathrm{f}})$ or equivalently $Q(\xi) = Q(\xi^{\mathrm{e}})$.

Proposition 3.10. *There exists a neigborhood $\mathfrak{V}$ of the equilibrium point ξ^{e} and a contant β such that the inequality $\sigma^{\mathrm{e}} - \sigma(h^{\mathrm{f}}, Y) \leq \beta\,\zeta$ holds on $\mathfrak{V} \cap \mathcal{X}$. That is, we have*

$$\forall \xi \in \mathfrak{V} \cap \{\, Q(\xi - \xi^{\mathrm{e}}) = 0 \,\}, \qquad \sigma(\xi^{\mathrm{e}}) - \sigma(\xi) \leq \beta\,\zeta(\xi).$$

Proof. We first note that

$$\zeta = \sum_{i \in R} \widehat{K}_i \Big(\langle M\nu_i^{\mathrm{d}}, \mu \rangle - \langle M\nu_i^{\mathrm{r}}, \mu \rangle \Big) \Big(\exp\langle M\nu_i^{\mathrm{d}}, \mu \rangle - \exp\langle M\nu_i^{\mathrm{r}}, \mu \rangle \Big), \tag{3.31}$$

where $\widehat{K}_i$, $i \in R$, are positive functions. As a consequence, there exists a neighorhood of $\xi^{\rm e}$ such that

$$\alpha \sum_{i\in R} \langle M\nu_i, \mu\rangle^2 \ \le \ \zeta, \tag{3.32}$$

for a positive constant α.

On the other hand we note that

$$\big\langle \mu - \mu^{\rm e}, Y - Y^{\rm e} \big\rangle = \Big\langle \int_0^1 (\partial_Y \mu)\big(Y^{\rm e} + \tau(Y - Y^{\rm e})\big)\, d\tau \ (Y - Y^{\rm e}),\ (Y - Y^{\rm e}) \Big\rangle,$$

and by using the negative definiteness of $R\partial_Y \mu = \partial_Y^2 \sigma$ over $M\mathcal{R}$ we obtain that in the neighborhood of $\xi^{\rm e}$ and on the simplex $\mathcal{X}$ we have

$$\|Y - Y^{\rm e}\|^2 \le \beta \Big| \big\langle \mu - \mu^{\rm e}, Y - Y^{\rm e} \big\rangle \Big|.$$

Denoting by Π the orthogonal projector onto $M\mathcal{R}$, this implies that

$$\|Y - Y^{\rm e}\| \le \beta \,\big\|\Pi(\mu - \mu^{\rm e})\big\|$$

since $Y - Y^{\rm e} = \Pi(Y - Y^{\rm e})$ on $\mathcal{X}$. Moreover, we also have

$$\sigma - \sigma^{\rm e} = \Big\langle \int_0^1 \int_0^\tau (\partial_Y^2 \sigma)\big(Y^{\rm e} + t(Y - Y^{\rm e})\big)\, dt\, d\tau\, (Y - Y^{\rm e}),\ (Y - Y^{\rm e}) \Big\rangle.$$

so that in the neiborhood of $Y^{\rm e}$ we have

$$\sigma^{\rm e} - \sigma \ \le \ \beta\, \|Y - Y^{\rm e}\|^2 \tag{3.33}$$

since we stay on the simplex $\mathcal{X}$ where $\partial_Y^2 \sigma$ is negative definite. Combining the above inequalities yields that

$$\sigma^{\rm e} - \sigma \ \le \ \beta\, \big\|\Pi(\mu - \mu^{\rm e})\big\|^2 \le \beta\zeta, \tag{3.34}$$

since

$$\big\|\Pi(\mu - \mu^{\rm e})\big\| \ \le \ \beta \sum_{i\in R} \langle M\nu_i, \mu - \mu^{\rm e}\rangle^2 = \beta \sum_{i\in R} \langle M\nu_i, \mu\rangle^2$$

and the proof is complete. ∎

A straightforward extension of the preceding proof yields the following inequality.

Proposition 3.11. *There exists a neigbornood $\mathfrak{V}$ of the equilibrium point $\xi^{\rm e}$ and a positive constant β such that*

$$\forall \xi \in \mathfrak{V}, \qquad \sigma(\mathfrak{v}^{\rm e}) - \sigma(\xi) \le \beta\, \zeta(\xi),$$

where $\mathfrak{v}^{\rm e}$ denotes the unique equilibrium point on $\xi + (0, M\mathcal{R})$.

3.6. Boundary equilibrium points

In Section 3.4, we have shown existence and uniqueness of the proper equilibrium ξ^{e} in the reaction simplex $\mathcal{X}$. From Proposition 3.6 we also know that any point in $\mathcal{X}$ where the chemical production terms vanish coincides with the unique equilibrium point. In this section, we further investigate the boundaries—with respect to the mass fractions—of the reaction simplex $\mathcal{X}$, which may hide points where the production terms vanish but which are not a global maximum of the entropy function over $\mathcal{X}$.

Definition 3.12. *A point (T, Y) with $T > 0$ and $Y \geq 0$, $Y \neq 0$ is said to be a boundary equilibrium point if $\omega(T, Y) = 0$ and if there exists at least a species $k \in S$ such that $Y_k = 0$.*

Note that it is always possible to construct reaction networks which have boundary equilibrium points, e.g., by adding a given species both as a reactant and as a product in each reaction of a given network.

Proposition 3.13. *Assume that (T, Y) is a boundary equilibrium point and define $S^+ = \{\, k \in S,\ Y_k > 0 \,\}$ and $S^0 = \{\, k \in S,\ Y_k = 0 \,\}$. Let us introduce the sets*

$$
\begin{aligned}
R^+ &= \{\ i \in R,\ \forall k \in S^0,\ \nu_{ki}^{\mathrm{d}} = 0 \text{ and } \nu_{ki}^{\mathrm{r}} = 0\ \},\\
R^0 &= \{\ i \in R,\ \exists k \in S^0,\ \nu_{ki}^{\mathrm{d}} > 0 \text{ or } \nu_{ki}^{\mathrm{r}} > 0\ \}.
\end{aligned}
$$

Then at (T, Y) we have $r_i = 0$, for all $i \in R$ and Y^+ is an equilibrium point of the S^+ mixture for the R^+ chemical network.

Proof. For any $k \in S^0$, the destruction rate vanish $Y_k \widehat{\mathcal{N}}_k = 0$, so that $\omega_k = 0$ implies that $\mathcal{P}_k = 0$. Since $\mathcal{P}_k$ is a sum of nonnegative terms, these terms must all vanish. This shows that $r_i = 0$ for any reaction $i \in R^0$. On the other hand, considering the submixture S^+, and the chemical subnetwork $\mathcal{R}^+$—which may be empty—we conclude that Y^+ is an equilibrium point of the submixture S^+. ■

Note that equilibrium points—which are interior to the simplex $\mathcal{X}$—only depend on the space spanned by the reaction vectors ν_i, $i \in R$. On the other hand, boundary equilibrium points depend on the effective values of the integer stoichiometric coefficients ν_i^{d} and ν_i^{r}, $i \in R$.

We now give a sufficient condition on stoichiometric coefficients which automatically eliminates boundary equilibrium points provided that all elements are present in the reactive mixture.

Definition 3.14. *A reaction network will said to have the decomposition chain property if for any $T > 0$ and any $Y \geq 0$, $Y \neq 0$, we have*

$$
\omega(T, Y) = 0 \text{ and } \exists k \in S,\ Y_k = 0 \quad \Longrightarrow \quad \exists l \in E,\ \langle Y, M^{-1}\mathcal{E}_l \rangle = 0.
$$

In other words, a boundary equilibrium point can only be obtained provided that one element is missing in the mixture at this point. The reaction scheme describing the combustion of hydrogen in air used in [GS92] has the decomposition chain property for instance. Heuristically, a reaction scheme has the decomposition chain property when sufficient three body recombination/decomposition reactions are taken into account. In this situation, the decomposition reactions form chains which link the largest molecules to the atomic elements and propagate the zero concentration property.

3.7. A global stability inequality

In the following, we assume that the reaction network and the conservation simplex are such that there are no boundary equilibrium points.

(H_6) There are no boundary equilibrium points in the set $\overline{\mathcal{X}}$ defined by

$$\overline{\mathcal{X}} = (Y^{\mathrm{f}} + M\mathcal{R}) \cap [0,\infty)^n \cap \{\, Y, \sum_{k\in S} Y_k h_k(0) < h^{\mathrm{f}} \,\}. \tag{3.35}$$

Under this assumption, we obtain a global stability inequality provided that the temperature is bounded.

Proposition 3.15. *Let $\mathfrak{a}$ and $\mathfrak{b}$ be positive constants such that $\mathfrak{a} < T^{\mathrm{e}} < \mathfrak{b}$. Then there exists $\epsilon > 0$ and $\beta > 0$ such that*

$$\forall \xi \in \{\, \mathfrak{a} \le T \le \mathfrak{b} \,\} \cap \{\, Y > 0 \,\} \cap \{\, Q(\xi - \xi^{\mathrm{e}}) \le \epsilon \,\} \qquad \sigma(\mathfrak{v}^{\mathrm{e}}) - \sigma(\xi) \le \beta\, \zeta(\xi),$$

where $\mathfrak{v}^{\mathrm{e}}$ denotes the unique equilibrium point on $\xi + (0, M\mathcal{R})$.

This proposition is proved by using a compacity argument. We already know from Proposition 3.11 that such an inequality holds near equilibrium points. We also know that the dissipation rate $\zeta(\xi)$ is positive for $Y > 0$ when ξ is not an equilibrium point. As a consequence, we only need to investigate the behavior of the chemical dissipation rate ζ near the boundary—with respect to zero mass fractions—of the set $\{\, \mathfrak{a} \le T \le \mathfrak{b} \,\} \cap \{\, Y > 0 \,\} \cap \{\, Q(\xi - \xi^{\mathrm{e}}) \le \epsilon \,\}$.

Lemma 3.16. *Consider the set $\{\, \mathfrak{a} \le T \le \mathfrak{b} \,\} \cap \{\, Y > 0 \,\} \cap \{\, Q(\xi - \xi^{\mathrm{e}}) \le \epsilon \,\}$ where $\mathfrak{a}$ and $\mathfrak{b}$ are positive constants such that $\mathfrak{a} < T^{\mathrm{e}} < \mathfrak{b}$. Then, there exists $\epsilon > 0$ such that the functional ζ is bounded from below by a positive constant near the zero mass fraction boundary.*

Proof. Assume that ϵ is small enough in such a way that there are no boundary equilibrium points in the set $Q(\xi - \xi^{\mathrm{e}}) \le \epsilon$. Consider then a boundary point $(T^{\mathrm{b}}, Y^{\mathrm{b}})$ such that Y^{b} is nonpositive. We can introduce the sets S^+, S^0, R^+, and R^0, as in Proposition 3.13. For Y in the neiborhood of Y^{b} and Y positive, we now write

$$\zeta = \frac{1}{RT}\Big(\sum_{k\in S^0} g_k m_k (Y_k \widehat{\mathcal{N}}_k - \mathcal{P}_k) - \sum_{k\in S^+} g_k m_k \omega_k \Big).$$

We have $-g_l m_l \mathcal{P}_l \ge 0$, $g_l Y_l \to 0$, and $-g_l \to +\infty$, for $l \in S^0$, when $Y \to Y^{\mathrm{b}}$. On the other hand, the quantities $g_l m_l \omega_l$, $l \in S^+$, remain bounded in the neiborhood of Y^{b}. As a consequence, if there exists $k \in S^0$ with $\mathcal{P}_k^{\mathrm{b}} > 0$, then ζ goes to $+\infty$ as $Y \to Y^{\mathrm{b}}$ since $-g_k m_k \mathcal{P}_k \to +\infty$. On the other hand, if $\mathcal{P}_k^{\mathrm{b}} = 0$ for all $k \in S^0$, then the term $-\sum_{k\in S^0} g_k m_k \mathcal{P}_k$ is nonnegative—although it may be arbitrary large—if Y is sufficiently close to Y^{b}, whereas the second term goes to

$$-\sum_{k\in S^+} g_k m_k \omega_k^+$$

where ω^+ only involve the chemical reactions of R^+ associated with the S^+ mixture. This limit is then positive otherwise Y^{b} would be a boundary equilibrium point from Proposition 3.6 applied to the submixture S^+. ∎

Note that for flame problems, the local inequality of Proposition 3.11 only involve high temperatures and small characteristic times. However, the global inequality of Proposition 3.15 involve low temperatures and large characteristic times depending on the lower bound $\mathfrak{a}$.

4. TRANSPORT COEFFICIENTS

In this section, we specify the properties of transport coefficients. These properties are deduced from previous work on diffusion matrices [Gio91] and from kinetic theory investigations of polyatomic reactive gas mixtures [EG94].

We first consider transport coefficients for nonnegative mass fractions. Indeed, although solutions of the flame equations will be shown to have positive mass fractions, we need to consider the case of zero mass fractions in order to achieve existence theorems. In particular, in the presence of zero mass fractions, the diffusion velocities cannot be defined [Gio91].

We then consider the more classical case of positive mass fractions. In this situation, we establish a new fundamental inequality about diffusion matrices which shows that the natural norm associated with multicomponent diffusion is a solution dependent weighted norm involving mass fractions at the denominator of the square of mass fraction gradients.

4.1. Mathematical assumptions on transport coefficients

The following properties of flux transport coefficients are derived from previous studies on diffusion matrices [Gio91] and kinetic theory investigations of polyatomic reactive gas mixtures [EG94]. In the appendix, we restate how these properties are also derived from Stefan-Maxwell-Boltzmann type equations.

(H_7) The flux diffusion coefficients C_{kl}, $k,l \in S$, the rescaled thermal diffusion ratios $\widetilde{\chi}_k$, $k \in S$, and the thermal conductivity λ are C^∞ functions of (T,Y) for $T > 0$ and $Y \geq 0$, $Y \neq 0$.

(H_8) The flux diffusion matrix $C = (C_{kl})_{k,l\in S}$ and the rescaled thermal difusion ratios $\widetilde{\chi}$ satisfy the mass constraints $N(C) = \mathbb{R}Y$, $R(C) = U^\perp$ and $\widetilde{\chi} \in \gamma^\perp$.

(H_9) The thermal conductivity λ is a positive function.

(H_{10}) For positive mass fractions, we define the matrix D by $D = (1/\rho)\mathcal{Y}^{-1}C$ where $\mathcal{Y} = \mathrm{diag}(Y_1, \ldots, Y_n)$. In this situation, the matrix $D = (D_{kl})_{k,l\in S}$ is symmetric positive semi-definite and its nullspace is spanned by $Y = (Y_1, \ldots, Y_n)^\star$. In particular, D is positive definite over $U^\perp$ where $U = (1, \ldots, 1)^\star$.

(H_{11}) For nonnegative mass fractions, we define $S^+ = \{\ k \in S,\ Y_k > 0\ \}$ and $S^0 = \{\ k \in S,\ Y_k = 0\ \}$, and we denote by Υ the permunation matrix associated with the reordering of S into (S^+, S^0). We then have the block structure

$$\Upsilon^\star C \Upsilon = \begin{pmatrix} C^{++} & C^{+0} \\ 0 & C^{00} \end{pmatrix},$$

and C^{00} is diagonal with positive entries. In addition, C^{++} is the flux diffusion matrix of the mixture associated with S^+ and defining D^{++} by $D^{++} = (1/\rho)(\mathcal{Y}^+)^{-1}C^{++}$, the matrix D^{++} is symmetric positive semidefinite and has nullspace $\mathbb{R}Y^+$ where Y^+ corresponds to the S^+ mixture, that it $Y = \Upsilon(Y^+, 0)$. Similarly, D^{++} is positive definite over the subspace $(U^+)^\perp$ where $U^+ \in \mathbb{R}^{n^+}$, $U^+ = (1, \ldots, 1)^\star$, and n^+ is the number of elements of S^+.

Note that the matrix C is singular since $CY = 0$ and not symmetric in general. Pressure dependencies of transport coefficients have not been written since p is constant. However, the only dependency is that D is inversely proportional to the pressure p so that ρD, C and λ only depend on (T, Y). As a consequence, properties (H_7)–(H_{11}) are uniformly valid for arbitrary gas mixtures. We also establish in the Appendix that D is always irreducible whereas C is irreducible if and only if $Y > 0$.

Properties (H_7)–(H_{11}) are more general than the assumptions considered in [GM98] where all mass fractions where assumed to be bounded away from zero. The situations where the diffusion process can be represented by a diagonal matrix have also been identified in [Gio91] and we refer to [Gio91] [EG94] and to the Appendix for more details. From assumptions (H_7)–(H_{11}), we now deduce various properties of transport coefficients and transport fluxes.

Lemma 4.1. *For $k, l \in S$, and $k \neq l$, the function D_{kl} admits a smooth extension to $T > 0$, and $Y \geq 0$, $Y \neq 0$. For $k \in S$, the function D_{kk} admits a smooth extention to $\{\, Y,\ Y \geq 0,\ Y_k > 0 \,\}$, and explodes like $1/Y_k$ as $Y_k \to 0$. In addition, we have $D_{kk} \geq 0$, and $D_{kk} = 0$ if and only if $Y_l = 0$ for $l \neq k$ and $Y_k > 0$.*

Proof. Consider a point Z such that $Z \geq 0$, $Z \neq 0$, and let Y be in the neighborhood of Z. When $Z_k > 0$, we have $Y_k > 0$ and from (H_{11}) we obtain $D_{kl}(T, Y) = C_{kl}(T, Y)/\big(\rho(T, Y)Y_k\big)$, so that $D_{kl}(T, Y)$ is smooth. Assume now that Z has at least a component such that $Z_k = 0$. We then consider $Y > 0$ in the neigborhood of Z and we define

$$\pi(Y) = \frac{Y - Y_k e_k}{1 - Y_k},$$

where e_k, $k \in S$, is the canonical basis of $\mathbb{R}^n$. We have of course $\pi(Y) \geq 0$ and $\pi(Y)_k = 0$. As a consequence, we obtain for $k \neq l$

$$C_{kl}(T, Y) - C_{kl}\big(T, \pi(Y)\big) = C_{kl}(T, Y) = \int_0^1 \Big\langle \partial_Z C_{kl}\big(T, yY + (1-y)\pi(Y)\big), Y - \pi(Y) \Big\rangle \, dy,$$

since $C_{kl}\big(T, \pi(Y)\big) = 0$ for $k \neq l$. However, since $Y - \pi(Y) = Y_k\big(e_k - \pi(Y)\big)$ we now obtain that

$$D_{kl}(T,Y) = \frac{C_{kl}(T,Y)}{\rho Y_k} = \frac{1}{\rho}\int_0^1 \Big\langle \partial_Z C_{kl}\big(T, yY + (1-y)\pi(Y)\big), e_k - \pi(Y)\Big\rangle \, dy,$$

so that $D_{kl}(T,Y)$ is a smooth function of (T,Y) for $T > 0$ and $Y \geq 0$, $Y \neq 0$, keeping in mind that C and π are smooth.

The smooth extension of D_{kk} to $\{\, Y,\ Y \geq 0,\ Y_k > 0 \,\}$ is also obvious from $D_{kk} = C_{kk}/\rho Y_k$. Moreover, the fact that D_{kk} explodes when $Y_k \to 0$ is a direct consequence of $C_{kk} > 0$ for $Y_k = 0$. Furthermore, for $Y_k > 0$ we obtain from (H_{11}) that $D_{kk} \geq 0$ since D^{++} is symmetric positive semi-definite. Finally, when $D_{kk} = 0$, we have $e_k^+ \in N(D^{++})$ and since $N(D^{++}) = \mathbb{R}Y^+$, we deduce that Y^+ is reduced to one element and the conversely. ∎

Note that C and D admits generalized inverses which naturally arise in the framework of the kinetic theory of gases or when investigating Stefan-Maxwell-boltzmann equations as shown in the Appendix [Gio90] [Gio91]. We now define the thermal diffusion coefficients θ_k, $k \in S$ and the partial thermal conductivity $\widehat{\lambda}$ in order to recover the more familiar expression (2.31)–(2.32).

Lemma 4.2. *Define the thermal diffusion ratios χ_k, $k \in S$, by*

$$\chi_k = \gamma_k \widetilde{\chi}_k, \qquad k \in S, \tag{4.1}$$

and the coefficients θ_k, $k \in S$, and $\widehat{\lambda}$ by the expressions

$$\theta_k = \frac{RT}{p}\sum_{l \in S} \frac{\widetilde{\chi}_l}{m_l} C_{lk}, \tag{4.2}$$

$$\widehat{\lambda} = \lambda + \frac{p}{T}\sum_{l \in S} \chi_l \theta_l. \tag{4.3}$$

Then the relations (2.31)–(2.32) hold, θ_k, $k \in S$, and $\widehat{\lambda}$ are smooth functions for $T > 0$ and $Y \geq 0$, $Y \neq 0$, and the partial thermal conductivity $\widehat{\lambda}$ is positive. In addition, when Y is positive, we have

$$\theta_k = \sum_{l \in S} D_{kl}\chi_l. \tag{4.4}$$

Proof. The smoothness of χ_k, $k \in S$, θ_k, $k \in S$, and $\widehat{\lambda}$ is a direct consequence of the definitions. From the properties of C and the symmety of D we also deduce that $Y_l C_{kl} = Y_k C_{lk}$, $k, l \in S$. Indeed, when Y_k and Y_l are both positive, we can write that $C_{kl}/Y_k = \rho D_{kl}$ and $C_{lk}/Y_l = \rho D_{lk}$ but D is symmetric by assumptions. On the other hand, when $Y_k = 0$ and $Y_l > 0$, we have $C_{kl} = 0$ by assumptions so that $Y_l C_{kl} = Y_k C_{lk}$, and the relation is trivial when $Y_k = Y_l = 0$. Now when Y is positive, we can write that $\widetilde{\chi}_l C_{lk} = \widetilde{\chi}_l \rho Y_l D_{lk}$ so that

$$\theta_k = \frac{RT}{p}\sum_{l \in S}\frac{\widetilde{\chi}_l}{m_l}\rho Y_l D_{lk} = \sum_{l \in S}\widetilde{\chi}_l \gamma_l D_{lk} = \sum_{l \in S} D_{kl}\chi_l,$$

which completes the proof. ∎

4.2. The fundamental diffusion inequality

The following inequality is essentially a consequence of [Gio91] and plays a fundamental role in the analysis.

Lemma 4.3. *Consider a fixed temperature T. Then there exists a positive constant α such that*

$$\forall Y > 0 \text{ with } \langle Y, U\rangle = 1, \quad \forall x \in U^{\perp} \qquad \langle \rho D x, x\rangle \;\geq\; \alpha\langle \mathcal{Y}^{-1}x, x\rangle, \tag{4.5}$$

where $\mathcal{Y} = \mathrm{diag}(Y_1, \ldots, Y_n)$.

Proof. Consider the quadratic form associated with the rescaled matrix

$$\begin{cases} \widehat{D}_{kk} = C_{kk}, & k \in S, \\ \widehat{D}_{kl} = \rho D_{kl}\sqrt{Y_k Y_l}, & k, l \in S, k \neq l. \end{cases}$$

Then $\widehat{D}$ is a continuous function over $Y \geq 0$, $\langle Y, U\rangle = 1$, from Lemma 4.1. Consider now the functional $(Y, x) \to \langle \widehat{D}(T, Y)x, x\rangle$ defined for $Y \geq 0$, $\langle Y, U\rangle = 1$, $\|x\| = 1$, and $\sum_{k\in S} x_k\sqrt{Y_k} = 0$. This continuous functional reaches a minimum over this compact set. Denoting by $(Y^{\mathrm{m}}, x^{\mathrm{m}})$ any point where the minimum is reached, by S^+ the set of positive mass fraction species at Y^{m} and by S^0 the set of zero mass fraction species at Y^{m}, we then have

$$\langle \widehat{D}(T, Y^{\mathrm{m}})x^{\mathrm{m}}, x^{\mathrm{m}}\rangle = \sum_{k,l\in S^+} \widehat{D}_{kl}(T, Y^{\mathrm{m}})x_k^{\mathrm{m}}x_l^{\mathrm{m}} \;+\; \sum_{k\in S^0} C_{kk}(T, Y^{\mathrm{m}})(x_k^{\mathrm{m}})^2.$$

Arguing by contradiction, we establish that $\langle \widehat{D}(T, Y^{\mathrm{m}})x^{\mathrm{m}}, x^{\mathrm{m}}\rangle$ is positive. First note that both terms are non negative from (H_{11}) and since $\widehat{D}_{kl} = \rho D_{kl}\sqrt{Y_k Y_l}$ for $k, l \in S^+$. Since we know that C_{kk}, $k \in S^0$, are positive, $\langle \widehat{D}(T, Y^{\mathrm{m}})x^{\mathrm{m}}, x^{\mathrm{m}}\rangle = 0$ implies that $x_k^{\mathrm{m}} = 0$, $k \in S^0$. On the other hand, we also have $\sum_{k\in S^+} x_k^{\mathrm{m}}\sqrt{Y_k} = 0$, and letting $z_k^{\mathrm{m}} = x_k^{\mathrm{m}}\sqrt{Y_k}$, $k \in S^+$, we then obtain

$$\langle \widehat{D}(T, Y^{\mathrm{m}})x^{\mathrm{m}}, x^{\mathrm{m}}\rangle = \sum_{k,l\in S^+} \rho D_{kl} z_k^{\mathrm{m}} z_l^{\mathrm{m}},$$

and $\sum_{k\in S^+} z_k^{\mathrm{m}} = 0$. When S^+ is reduced to one element, we then have $x_k^{\mathrm{m}} = 0$, for $k \in S^+$ since there is only one term in the sum $\sum_{k\in S^+} z_k^{\mathrm{m}} = 0$. On the other hand, when there are more than two elements in S, we know that D is positive definite over $U^{\perp}$ which implies that $z_k^{\mathrm{m}} = 0$, $k \in S^+$, and thus that $x_k^{\mathrm{m}} = 0$, $k \in S^+$. Finally, we have shown that $x^{\mathrm{m}} = 0$ which contradicts $\|x^{\mathrm{m}}\| = 1$ and the proof is complete. ■

Note that the properties of ρD—including the fundamental inequality—can also be rewritten in terms of the flux diffusion matrix C.

Corrolary 4.4. *The flux diffusion matrix C is such that $C\mathcal{Y}$ is symmetric positive semi-definite. Moreover, for any fixed temperature T, there exists a positive constant α such that*

$$\forall Y \geq 0, \text{ with } \langle Y, U\rangle = 1, \quad \forall x \in \mathbb{R}^n, \text{ with } \mathcal{Y}x \in U^{\perp}, \qquad \langle C\mathcal{Y}x, x\rangle \;\geq\; \alpha\langle \mathcal{Y}x, x\rangle. \tag{4.6}$$

In addition, for any $k \in S$, we have $C_{kk} \geq 0$, and $C_{kk} = 0$ if and only if $Y_l = 0$ for $l \neq k$ and $Y_k > 0$.

4.3. Uniform temperature scaling

We now focus on the global temperature dependency of transport coefficients. More specifically, we assume a common temperature scaling for all transport coefficients. This common temperature scaling is suggested by the kinetic theory provided that the same type of interaction potential is used for each pair of molecules.

(H_{12}) There exists a positive function $\varphi(T)$ defined for $T > 0$ such that the rescaled properties $D^0(T,Y) = \rho D/\varphi(T)$, $C^0(T,Y) = C/\varphi(T)$, $\lambda^0(T,Y) = \lambda/\varphi(T)$, and $\widetilde{\chi}^0 = \widetilde{\chi}$ admit a continuous extension to $T \in [0,\infty]$, $Y \geq 0$, $Y \neq 0$, satisfying (H_8)–(H_{11}).

Note that $\varphi = 1$ is generally used in mathematics whereas various functions φ are suggested by the kinetic theory of gases, depending on the interaction potentials between pairs of molecules. For a rigid sphere interaction potential, we have for instance $\varphi = T^{1/2}$. For point centers of repulsion, we have $\varphi = T^{(\nu-4)/2\nu}$ where ν varies from $\nu = 4$—Maxwell molecules—to infinity and the temperature dependence varies respectively betwen $\varphi = 1$ and $\varphi = T^{1/2}$ [FK72]. Small values of ν corresponds to soft molecules whereas large values of ν corresponds to hard molecules, and for $\nu \to \infty$ we recover the hard sphere model. For Lennard-Jones or Stockmayer potentials the existence of φ is a consequence of the Mason and Monchick tables for collision integral ratios [FK72]. In addition, from definitions (4.2) and (4.3) the quantities $\widehat{\lambda}/\varphi(T)$ and $\rho\theta/\varphi(T)$ also admits a continuous extension. By a straightforward adaptation of Lemma 4.3 we obtain the following fundamental result.

Corrolary 4.5. *There exists a positive constant α such that*

$$\forall T > 0,\ \forall Y > 0,\ \langle Y, U\rangle = 1, \qquad \forall x \in U^{\perp} \qquad \langle \rho D x, x\rangle \ \geq\ \alpha\, \varphi(T)\, \langle \mathcal{Y}^{-1}x, x\rangle. \quad (4.7)$$

4.4. The matrix $\mathcal{L}$

The transport fluxes ϕ are naturally expressed in terms of the gradients of the state variables T and Y. In order to manipulate the conservation equations, we need to express ϕ in terms of the gradients of the conservative variables h and Y [GM98].

Definition 4.6. *Define the matrix $\mathcal{L}$ by*

$$\mathcal{L} = \begin{pmatrix} 1 & \widehat{h}_1,\dots,\widehat{h}_n \\ 0 & I \end{pmatrix} \begin{pmatrix} \lambda/c_p & 0 \\ C\chi/c_pT & C\, d_Y\gamma \end{pmatrix} \begin{pmatrix} 1 & -h_1,\dots,-h_n \\ 0 & I \end{pmatrix}, \qquad (4.8)$$

where $\widehat{h}_k = h_k + RT\widetilde{\chi}_k/m_k$, $k \in S$. Then we have

$$\phi = -\mathcal{L}\xi', \qquad (4.9)$$

and $\mathcal{L}$ is such that $R(\mathcal{L}) = \mathcal{U}^\perp$, where $\mathcal{U} = (0, U)^\star$, and $N(\mathcal{L}) = \mathbb{R}\xi$.

Proof. A straightforward calculation directly yields the expression of $\mathcal{L}$ and the identity $\phi = -\mathcal{L}\xi'$. From this expresion, the relation

$$d_Y\gamma = \frac{1}{\langle Y, U\rangle}\Big(I - \frac{X \otimes U}{\langle Y, U\rangle}\Big)\, A$$

where $X = (X_1, \ldots, X_n)^\star$, and the identity $\langle Y, U\rangle = \langle X, U\rangle$, we then obtain that $R(\mathcal{L}) = \mathcal{U}^\perp$, and $N(\mathcal{L}) = \mathbb{R}\xi$. Indeed, we have $C(d_Y\gamma)\, x = 0$ if and only if $(d_Y\gamma)\, x = 0$ since $R(d_Y\gamma) = U^\perp$ and $N(C) \cap U^\perp = \{0\}$. On the other hand, thanks to $AY = X$, we have $(d_Y\gamma)\, x = 0$ if and only if $Ax \in \mathbb{R}X$, that is, if and only if $x \in \mathbb{R}Y$. ■

The following proposition is a direct consequence of classical results concerning generalized inverses with prescribed range and nullspace [BG74] [EG94] [EG97].

Proposition 4.7. *Assume that $T > 0$ and $Y \geq 0$, $Y \neq 0$. Then there exists a unique matrix $\mathcal{L}^\sharp$ such that $\mathcal{L}\,\mathcal{L}^\sharp\mathcal{L} = \mathcal{L}$, $\mathcal{L}^\sharp\mathcal{L}\,\mathcal{L}^\sharp = \mathcal{L}^\sharp$, $N(\mathcal{L}^\sharp) = N(\mathcal{L})$ and $R(\mathcal{L}^\sharp) = R(\mathcal{L})$. The matrix $\mathcal{L}^\sharp$ is a smooth function of $T > 0$ and $Y \geq 0$, $Y \neq 0$, and $\mathcal{L}\,\mathcal{L}^\sharp = \mathcal{L}^\sharp\mathcal{L}$ is the oblique projector onto $R(\mathcal{L})$ parallel to $N(\mathcal{L})$.*

Finally, we investigate how the diffusion flux $\mathcal{F}_k$ of the k^{th} species behaves when Y_k goes to zero. A straightforward calculation indeed yields the following result.

Lemma 4.8. *The diffusion flux $\mathcal{F}_k$ of the k^{th} species can we written in the form*

$$\mathcal{F}_k = -d_k Y_k' - Y_k \pi_k, \tag{4.10}$$

where

$$d_k = \frac{C_{kk} A_{kk}}{\langle Y, U\rangle}, \tag{4.11}$$

and

$$\pi_k = \frac{C_{kk}}{m_k}\Big(\sum_{l\in S}\frac{Y_l}{m_l}\Big)^{-2}\sum_{\substack{l\in S\\ l\neq k}}\frac{X_l'}{m_l} + \frac{C_{kk}}{m_k}\widetilde{\chi}_k\Big(\sum_{l\in S}\frac{Y_l}{m_l}\Big)^{-1}\frac{T'}{T} + \sum_{\substack{l\in S\\ l\neq k}}\rho D_{kl}\big(\gamma_l' + \gamma_l\widetilde{\chi}_l(T'/T)\big), \tag{4.12}$$

so that the nondiagonal part of the multicomponent flux $\mathcal{F}_k$ vanishes for $Y_k = 0$. Moreover we always have $d_k \geq 0$, and $d_k = 0$ if and only if $Y_l = 0$ for $l \neq k$ and $Y_k > 0$. In particular, whenever $\langle Y, U\rangle = 1$, d_k is positive and bounded away from zero when $0 \leq Y_k \leq \delta$ for any $\delta < 1$.

4.5. The entropy conservation equation

In this section, we establish the entropy conservation equation which plays a fundamental role in the analysis. The existence of an entropy function is an important property of the system [GM98] and will often be used in order to obtain a priori estimates.

Lemma 4.9. *Assume that (T, Y) is a regular solution of the flame equations and that T and Y are positive. Then the entropy function $\sigma(h, Y) = s(T, Y)$ satisfies the equation*

$$c\sigma' + \langle \partial_\xi \sigma, \phi \rangle' = \kappa, \tag{4.13}$$

where the dissipation rate κ is given by

$$\kappa = \lambda (T'/T)^2 + \frac{p}{T} \sum_{k,l \in S} D_{kl} \big(\gamma_k' + \chi_k (T'/T)\big) \big(\gamma_l' + \chi_l (T'/T)\big) - \sum_{k \in S} \frac{g_k m_k \omega_k}{T}. \tag{4.14}$$

Proof. We have $\sigma' = \langle \partial_\xi \sigma, \xi' \rangle$ so that from the conservation equations we obtain

$$c\sigma' = \langle \partial_\xi \sigma, -\phi' + w \rangle = -\langle \partial_\xi \sigma, \phi \rangle' + \kappa,$$

where κ is defined by

$$\kappa = \big\langle (\partial_\xi \sigma)', \phi \big\rangle + \langle \partial_\xi \sigma, w \rangle = \big\langle (\partial_\xi^2 \sigma) \xi', \phi \big\rangle + \langle \partial_\xi \sigma, w \rangle.$$

We now obtain that $\langle \partial_\xi \sigma, w \rangle = R\zeta$ is the entropy production rate due to chemistry and that

$$\big\langle (\partial_\xi^2 \sigma) \xi', \phi \big\rangle = \big\langle (\partial_\xi \sigma)', \phi \big\rangle = -\Big(\frac{1}{T}\Big)' q - \sum_{k \in S} \Big(\frac{g_k}{T}\Big)' \mathcal{F}_k,$$

since $\partial_h \sigma = (1/T)$ and $\partial_{Y_k} \sigma = -g_k/T$ from Lemma 3.3. Using

$$\Big(\frac{g_k}{T}\Big)' = -\frac{h_k}{T^2} + \frac{R}{m_k} \frac{\gamma_k'}{\gamma_k},$$

we obtain after a little algebra

$$\big\langle (\partial_\xi^2 \sigma) \xi', \phi \big\rangle = -\frac{(q - \sum_{k \in S} h_k \mathcal{F}_k) T'}{T^2} - \sum_{k \in S} \frac{R}{m_k} \frac{\gamma_k'}{\gamma_k} \mathcal{F}_k,$$

which can be rewritten, by using the expression (2.28) of the heat flux, in the form

$$\big\langle (\partial_\xi^2 \sigma) \xi', \phi \big\rangle = \frac{\big(\lambda T' - RT \sum_{k \in S} (\widetilde{\chi}_k / m_k) \mathcal{F}_k\big) T'}{T^2} - \sum_{k \in S} \frac{R}{m_k} \frac{\gamma_k'}{\gamma_k} \mathcal{F}_k.$$

This yields

$$\big\langle (\partial_\xi^2 \sigma) \xi', \phi \big\rangle = \lambda (T'/T)^2 - \sum_{k \in S} \frac{R}{m_k} \frac{\gamma_k' + \chi_k (T'/T)}{\gamma_k} \mathcal{F}_k,$$

and finally

$$\big\langle (\partial_\xi^2 \sigma) \xi', \phi \big\rangle = \lambda (T'/T)^2 + \frac{p}{T} \sum_{k \in S} D_{kl} \big(\gamma_k' + \chi_k (T'/T)\big) \big(\gamma_l' + \chi_l (T'/T)\big),$$

and the proof is complete. ∎

Note that Equation (4.13) is only valid when the mass fractions Y_k, $k \in S$, are positive. Since $\langle (\partial_\xi^2 \sigma)\xi', \phi\rangle$ is the nonreactive part of the dissipation rate, the hessian matrix may also be seen as a metric which correlates the flux ϕ and the gradient ξ', but this metric is singular for zero mass fractions. The entropy equation also shows that the natural norm for multicomponent diffusion is not the H^1 Sobolev norm but involves mass fractions at the denominator from (4.7).

5. FIRST PROPERTIES

In this section, we establish that each solution of the anchored flame problem can be extended uniquely into a solution on the full line satisfying (2.38). Conversely, we establish that the reduction to $[0, \infty)$ of any solution on $(-\infty, \infty)$ is a solution of the anchored flame problem.

5.1. Preliminaries

A triplet (T, Y, c) such that T and Y are $C^2[0, \infty)$, such that $T > 0$, $Y \geq 0$, $Y \neq 0$, and $c > 0$, and which satisfies pointwise the governing equations and boundary conditions (2.35)–(2.37), will be said to be a solution of the anchored flame problem. Similarly, a triplet (T, Y, c) such that T and Y are $C^2[0, \infty) \cap C^2[-\infty, 0]$ and $C^1(-\infty, \infty)$, such that $T > 0$, $Y \geq 0$, $Y \neq 0$, and $c > 0$, and which satisfies pointwise the governing equations and boundary conditions (2.35) (2.38) and (2.37), will be said to be a solution on the full line.

We first establish some a priori estimates for any solution of the anchored flame problem which will be further needed.

Lemma 5.1. *Let (T, Y, c) be a solution of the anchored flame problem. Then the mass fractions are positive $Y > 0$ and sum up to unity $\langle U, Y\rangle = 1$.*

Proof. Let (T, Y, c) be a solution of the anchored flame problem. We first deduce from the species equations that $c\langle U, Y\rangle' = 0$ since $R(\mathcal{C}) = U^\perp$ and $M\omega \in U^\perp$. This shows that $\langle U, Y\rangle$ is constant, and this constant is equal to unity since the boundary condition (2.36) implies $\langle U, Y\rangle = \langle U, Y^{\mathrm{f}}\rangle = 1$.

Aguing by contradiction, we now establish that $Y(0) > 0$. We assume that there exists $k \in S$ such that $Y_k(0) = 0$. Then, using Lemma 4.10 and the boundary condition $c(Y_k(0) - Y_k^{\mathrm{f}}) + \mathcal{F}_k(0) = 0$, we deduce that

$$Y_k'(0) = -\frac{cY_k^{\mathrm{f}}}{d_k(0)}.$$

If $Y_k^{\mathrm{f}} > 0$, then Y is negative on an interval of the form $(0, \epsilon)$ with $\epsilon > 0$, which contradicts the assumptions that (T, Y, c) is a solution of the anchored flame problem. Hence, if $Y_k(0) = 0$, we must have $Y_k^{\mathrm{f}} = 0$ and consequently we have $Y_k'(0) = 0$. By expanding the derivative $\mathcal{F}_k'$ in (2.1) and then letting $x = 0$, we further obtain that

$$d_k Y_k'' = -m_k \mathcal{P}_k,$$

since $\mathcal{N}_k = 0$ for $Y_k = 0$. If $\mathcal{P}_k > 0$ then $Y_k''(0) < 0$ which is imposible since Y is assumed to be a solution of the anchored flame problem. Hence we have $\mathcal{P}_k = 0$ at $x = 0$ and $Y_k''(0) = 0$.

We now introduce the set $\mathcal{I} = \{\ k \in S,\ Y_k(0) = 0\ \}$ and from the preceding discussion we know that

$$\forall k \in \mathcal{I},\ Y_k(0) = 0,\ Y_k'(0) = 0,\ Y_k''(0) = 0,\ \mathcal{P}_k(0) = 0. \tag{5.1}$$

As a consequence, any reaction creating a species $\mathcal{S}_k$ with $k \in \mathcal{I}$ needs at least one species $\mathcal{S}_i$ with $i \in \mathcal{I}$ as a reactant, otherwise one would get a positive production term $\mathcal{P}_k$. This shows that the mass fractions Y_k, $k \in \mathcal{I}$, are factorized in the production terms ω_l, $l \in \mathcal{I}$. Now the mass fractions Y_k, $k \in \mathcal{I}$, are solutions of the system

$$cY_k' = \Big(d_k(x)Y_k' + Y_k\pi_k(x)\Big)' + m_k\omega_k, \qquad k \in \mathcal{I},$$

where d_k and π_k are defined in Lemma 4.10, and the mass fractions vanish at $x = 0$ with their first derivatives. However, this system has a locally unique solution by virtue of the Cauchy-Lipchitz theorem. Since this system also admits the trivial solution, we conclude that locally, we have $Y_k(x) = 0$, for $x \in [0, \epsilon]$, and $k \in \mathcal{I}$. An easy argument then yields that $Y_k(x) = 0$, for $x \in [0, \infty)$, and $k \in \mathcal{I}$, contradicting that $Y_k(\infty) = Y_k^{\mathrm{e}} > 0$.

We now have to show that $Y > 0$ over $(0, \infty)$. Arguing by contradiction, assume that there exists a point $x_0 > 0$ and $k \in S$ such that $Y_k(x_0) = 0$. We may also assume that x_0 is the smallest point where a species vanishes. We then have $Y_k'(x_0) \leq 0$ by construction. If $Y_k'(x_0) < 0$, we obtain a contradiction with the fact that Y is nonnegative. On the other hand, if $Y_k'(x_0) = 0$, we can then argue as above and show that Y_k is zero in the neiborhood of x_0, contradicting the definition of x_0 and the proof is complete. ∎

5.2. Reduction to a problem on $[0, \infty)$

Proposition 5.2. *Let (T, Y, c) be a solution on the full line. Then we have*

$$c\big(\xi(x) - \xi^{\mathrm{f}}\big) + \phi(x) = 0, \qquad x \leq 0, \tag{5.2}$$

and the reduction of (T, Y, c) to $[0, \infty)$ is a solution of the anchored flame prolem.

Proof. From the governing equations we have $\langle Y', U\rangle = 0$ so that $\langle Y, U\rangle$ is a constant and this constant is unity from $\langle Y^{\mathrm{f}}, U\rangle = 1$. From the governing equations, the quantity $c\xi+\phi = c\xi - \mathcal{L}\xi'$ is a constant over $(-\infty, 0]$, say $c\xi - \mathcal{L}\xi' = u$. Since $\xi' \in \mathcal{U}^\perp$ we can write that $\xi' = \mathcal{L}^\sharp(c\xi - u)$. This shows that ξ' admits a limit as $x \to -\infty$ since $\xi(-\infty) = \xi^{\mathrm{f}}$ and this limit can only be zero. As a consequence, we must have $u = c\xi^{\mathrm{f}}$ and we conclude that $c\xi + \phi = c\xi^{\mathrm{f}}$ over $(\infty, 0]$ so that the restriction to $[0, \infty)$ of (T, Y, c) is a solution of the anchored flame problem. ∎

5.3. Extention to $(-\infty, 0)$

In this section, we establish that any solution of the anchored flame problem can be extended over $(-\infty,0)$. However, we will further need to extend any solution obtained on bounded domain for a priori estimates. As a consequence, we investigate the extension starting from any positive species at the origin and will apply this result to both situations.

Proposition 5.3. *Let $Y^0>0$ and $c>0$ be given such that $\langle Y^0,U\rangle=1$, and let $\xi^0=(h(T^{\mathrm{i}},Y^0),Y^0)$. Then there exists a unique solution (T,Y) to the flame equations over $(-\infty,0]$ such that $\xi(0)=\xi^0$ and $\xi(-\infty)=\xi^{\mathrm{f}}$. Furthermore, this solution satisfies (5.2) and there exist are positive constants $\mathfrak{a}$ and $\mathfrak{b}$ such that $0<\mathfrak{a}\leq T\leq\mathfrak{b}$. In addition, the mass fraction are positive, satisfy $\langle Y,U\rangle=1$, and the integral over $(-\infty,0]$ of the dissipation rate κ is finite and given by*

$$\int_{-\infty}^{0}\kappa\,dx=c\Big(\sigma(0)-\sigma^{\mathrm{f}}-\big\langle\partial_\xi\sigma(0),\xi(0)-\xi^{\mathrm{f}}\big\rangle\Big). \tag{5.3}$$

Proof. We have established in the proof of Proposition 5.2 that any solution of the flame equations such that (2.38) holds must satisfy (5.2). As a consequence, any such solution satisfies the ordinary differential equation

$$z'=c\mathcal{L}^\sharp(z-\xi^{\mathrm{f}}), \tag{5.4}$$

with initial value $\xi(0)=\xi^0$. Now such a solution locally exists and is unique from the Cauchy-Lipchitz theorem so that we only have to extend this solution over $(-\infty,0]$.

Consider such a a solution over $[x_0,0]$ and, locally, the species are positive. It is easily checked that $\langle Y,U\rangle=1$ so that the mass fractions are bounded. From the govening equations, we obtain, after a little algebra, that

$$\sum_{k\in S}Y_k^{\mathrm{f}}(h_k-h_k^{\mathrm{f}})-\lambda T'+RT\sum_{k\in S}\frac{\widetilde{\chi}_k}{m_k}Y_k^{\mathrm{f}}=0.$$

Consider any x_1 where T reaches its minimum over $[x_0,0]$. If $T(x_1)\leq T^{\mathrm{f}}$ then we must either have $T'(x_1)=0$ when $x_1\in(x_0,0)$ or $T'(x_1)\geq 0$ when $x_0=x_1$, $x_1=0$ being excluded since $T^{\mathrm{f}}<T^{\mathrm{i}}$. As a consequence, if $T(x_1)\leq T^{\mathrm{f}}$ then

$$\sum_{k\in S}Y_k^{\mathrm{f}}\Big(h_k\big(T(x_1)\big)-h_k\big(T^{\mathrm{f}}\big)\Big)+RT(x_1)\sum_{k\in S}\frac{\widetilde{\chi}_k}{m_k}Y_k^{\mathrm{f}}\geq 0.$$

Keeping in mind that $T(x_1)\leq T^{\mathrm{f}}$, this yields that

$$\underline{c}_p\big(T(x_1)-T^{\mathrm{f}}\big)+T(x_1)\overline{\chi}\geq 0,$$

where $\overline{\chi}\geq 0$ is such that

$$R\sum_{k\in S}\frac{|\widetilde{\chi}_k|}{m_k}Y_k^{\mathrm{f}}\leq\overline{\chi}.$$

We have thus shown that

$$T\geq\mathfrak{a}=\frac{\underline{c}_p\,T^{\mathrm{f}}}{\underline{c}_p+\overline{\chi}},$$

so that T is uniformly bounded from below.

This method cannot be used, however, in order to derive an upper bound for T, unless the thermal diffusion factors are small quantities. In particular, when $\widetilde{\chi} = 0$, one easily shows that $T^{\rm f} \leq T \leq T^{\rm i}$. For the general case $\widetilde{\chi} \neq 0$, we integrate the entropy conservation equation over $[x, 0]$

$$c(\sigma(0) - \sigma) + \langle \partial_\xi \sigma, \phi\rangle(0) - \langle \partial_\xi \sigma, \phi\rangle = \int_x^0 \kappa \, du,$$

so that from $c(\xi - \xi^{\rm f}) + \phi = 0$ we obtain that

$$c\left(\sigma - \sigma^{\rm f} - \langle \partial_\xi \sigma, \xi - \xi^{\rm f}\rangle\right) = c\left(\sigma(0) - \sigma^{\rm f} - \langle \partial_\xi \sigma(0), \xi(0) - \xi^{\rm f}\rangle\right) - \int_x^0 \kappa \, du. \tag{5.5}$$

As a consequence, the functional $\sigma - \sigma^{\rm f} - \langle \partial_\xi \sigma, \xi - \xi^{\rm f}\rangle$ is increasing over $[x_0, 0]$ and nonnegative by concavity. After a little algebra, we easily evaluate this functional and deduce that

$$\frac{h^{\rm f}}{T} - \sum_{k\in S} Y_k^{\rm f} \frac{h_k(T)}{T} + \sum_{k\in S} Y_k^{\rm f} s_k(T, Y) \leq \sigma(0) - \langle \partial_\xi \sigma(0), \xi(0) - \xi^{\rm f}\rangle.$$

Using now the lower bound for T and the expression (2.15) we get that

$$\sum_{k\in S} Y_k^{\rm f} \Big(-\frac{R}{m_k} \log X_k + \int_{\mathfrak{a}}^T \frac{c_{pk}(t)}{t} dt \Big) \leq b,$$

where b is a positive constant wich depends only on the data and on ξ^0. This implies that $T \leq \mathfrak{b}$ over $[x_0, 0]$ where $\mathfrak{b}$ is independent of x_0, and that Y_k is bounded away from 0 when k is such that $Y_k^{\rm f} > 0$.

We now consider a maximal solution defined on $(x_1, 0]$ and we argue by contradiction by assuming that x_1 is finite. In this situation, from the preceding estimates, and the smoothness of the coefficients, ξ' remain finite in the neighborhood of x_1 so that the limit $\xi(x_1)$ exists and also $\xi'(x_1)$. As a consequence, if x_1 is finite, we have either $Y > 0$ and the solution can be extended, contradicting the definition of x_1, or there exists $k \in S$ such that $Y_k(x_1) = 0$. Since $\forall x \in (x_1, 0]$, $\forall k \in S$, $Y_k(x) > 0$, we have $Y_k'(x_1) \geq 0$ by construction and from (5.2) and (4.10)

$$Y_k'(x_1) = -\frac{cY_k^{\rm f}}{\rho d_k}.$$

When $Y_k^{\rm f} > 0$, this yields $Y_k'(x_1) < 0$ and we have obtained a contradiction. On the other hand, if $Y_k^{\rm f} = 0$, this yields that $Y_k'(x_1) = 0$ and thus that $Y_k = 0$ by the Cauchy Lipchitz theorem applied to $z = Y_k$ solution of

$$cz = d_k(x) z' + z\pi_k(x),$$

where d_k and π_k are defined in Lemma 4.10. We then obtain $Y_k = 0$ in the neighborhood of x_1, contradicting the definition of x_1. As a consequence, the solution can be extended over the half line $(-\infty, 0]$ and the temperature and mass fractions remain positive.

From the identity (5.5) we also obtain that the integral of the dissipation rate κ remain finite. Using now the estimate $\langle \phi, \phi \rangle \leq \beta\kappa$ where β is a positive constant, and $\phi = -c(\xi - \xi^{\mathrm{f}})$, we obtain that $\xi - \xi^{\mathrm{f}} \in H^1(-\infty, 0)$ and thus $\xi(-\infty) = \xi^{\mathrm{f}}$. This now show that

$$c\Big(\sigma(0) - \sigma^{\mathrm{f}} - \langle \partial_\xi \sigma(0), \xi(0) - \xi^{\mathrm{f}} \rangle\Big) = \int_{-\infty}^{0} \kappa\, dx,$$

and that the upper bound for T is finally controled by the data and the integral of the reduced dissipation rate κ/c. ∎

We can now apply this result to any solution of the anchored flame problem since we know that $Y(0) > 0$.

Corrolary 5.4. *Let (T, Y, c) be a solution of the anchored flame problem. Then this solution has a unique extension over $(-\infty, 0)$ such that (2.36) holds. Moreover, this solution satisfies (5.2) and the mass fractions are positive over $(-\infty, 0]$ and the identity (5.3) holds.*

6. EXISTENCE ON A BOUNDED DOMAIN

In this section, we establish an existence theorem on a bounded domain $[0, a]$. In the next section, we will let $a \to \infty$ and obtain a solution of the anchored flame problem.

6.1. Preliminaries

For technical reasons, we need to extend the domain of definition of the equations coefficients. To this purpose, we introduce the definition

$$\widetilde{Y} = \begin{cases} Y^+, & \text{if } \langle Y, U \rangle \geq 1, \\ Y^+ + \dfrac{1 - \langle Y, U \rangle}{n}\, U, & \text{if } \langle Y, U \rangle \leq 1. \end{cases} \tag{6.1}$$

We note that we have $\widetilde{Y} \geq 0$ and $\langle \widetilde{Y}, U \rangle \geq 1$ for any $Y \in \mathbb{R}^n$. In addition, whenever $\langle Y, U \rangle = 1$, we have $\widetilde{Y} = Y^+$ so that both properties $Y \geq 0$ and $\langle Y, U \rangle = 1$ imply that $\widetilde{Y} = Y$. For a fixed point formulation, the transport coefficients, the thermodynamic properties and the chemical production rates can be taken to be functions of $(T, \widetilde{Y})$, and are then defined for $T > 0$ and any $Y \in \mathbb{R}^n$. In order to avoid too complex notation, we will denote by $\widetilde{\psi}$ the function $\psi(T, \widetilde{Y})$ associated with any function $\psi(T, Y)$.

In order to obtain a suitable fixed point formulation, it is preferable to control the temperature and thus to use (T, Y, c) as an unknown, rather than using the specific enthalpy h. However, the enthalpy equation is simpler than the temperature equation and can be integrated once, making use of the flux boundary conditions. In order to keep both advantages, we will solve the equations in the form

$$\xi' = \mathcal{L}^\sharp\Big(c(\xi - \xi^{\mathrm{f}}) - \int_0^x w(u)\, du\Big),$$

with h' replaced by $c_pT' + \sum_{k\in S} h_k(T)Y_k'$ and h by $\int_0^T c_p du + \sum_{k\in S} h_k^0 Y_k$. That is, we will solve the problem in the form

$$\Big(c_pT' + \sum_{k\in S} h_k(T)Y_k',\, Y'\Big)^\star = \mathcal{L}^\sharp\Big(c\Big(\int_0^T c_p dx + \sum_{k\in S} h_k^0 Y_k,\, Y\Big)^\star - c\xi^{\mathrm{f}} - \int_0^x w(u)\, du\Big),$$

with the backward initial conditions $\xi(a) = \xi^{\mathrm{e}}$ with the extra relation $T(0) = T^{\mathrm{i}}$ used as an equation for the eigenvalue c.

In order to establish the existence of a solution, we will use the Leary-Schauder topological degree theory and the homotopy invariance of the degree. We will first eliminate the chemistry in a first homotopy path, and then simplify thermodynamic properties and transport fluxes along a second homotopy path. Evaluation of the resulting degree will conclude the existence proof.

6.2. A fixed point formulation

We consider the Banach space

$$\mathcal{B} = \big(C^1[0,a]\big)^{n+1} \times \mathbb{R}, \tag{6.2}$$

and the open set $\mathcal{O} \subset \mathcal{B}$

$$\mathcal{O} = \{\ (T, Y, c) \in \mathcal{B},\ T > 0,\ c > 0\ \}. \tag{6.3}$$

We introduce the operator

$$\mathcal{K}_\tau\ :\ \mathcal{O} \longrightarrow \mathcal{B},$$

defined by

$$\mathcal{K}_\tau(T, Y, c) = \Big(t, y, c + t(0) - T^{\mathrm{i}}\Big), \tag{6.4}$$

where (t, y) are solutions of the system

$$\Big(\widetilde{c}_pt' + \sum_{k\in S} h_k y_k', y'\Big)^\star = \widetilde{\mathcal{L}}^\sharp\Big(c\Big(\int_0^t \widetilde{c}_p dx + \sum_{k\in S} h_k^0 y_l, y\Big)^\star - c\xi^{\mathrm{f}} - \tau\int_0^x \widetilde{w}(u)\, du\Big), \tag{6.5}$$

with the backward initial conditions

$$t(a) = T^{\mathrm{e}}, \qquad y(a) = Y^{\mathrm{e}}. \tag{6.6}$$

Note that nonlinearities are taken as functions of $(T, \widetilde{Y})$ in the homotopy path and that for $\tau = 0$ the chemistry source terms vanish. The extra left boundary conditions $T(0) = T^{\mathrm{i}}$ is also used as an equation for the eigenvalue c.

Proposition 6.1. *The operator $\mathcal{K}_\tau$ from $\mathcal{O}$ to $\mathcal{B}$ is well defined.*

Proof. Consider the backward ordinary differential equation with initial condition $(t, y)(a) = (T^{\mathrm{e}}, Y^{\mathrm{e}})$. This system of ordinary differential equations admits a unique solution from the Cauchy-Lipchitz theorem, keeping in mind that the right member is bounded by an affine function of (t, y) [Bou76]. ■

We also have the following property which allows us to use the homotopy invariance of the degree.

Lemma 6.2. *Let B be a closed bounded set in $\mathcal{O}$ and let $\mathcal{K} : [0,1] \times B \to \mathcal{B}$ be the map defined by $\mathcal{K}\big(\tau, (T, Y, c)\big) = \mathcal{K}_\tau(T, Y, c)$. Then $\mathcal{K}$ is a compact map.*

Proof. We establish from the definition of (t, y) that for $\big(\tau, (T, Y, c)\big) \in [0,1] \times B$, t, y, t', and y' are uniformly bounded and that t' and y' are uniformly Lipchitzian. This implies that the range of $\mathcal{K}$ is relatively compact and that $\mathcal{K}$ is continuous by uniqueness of the solution of (6.5)–(6.6). ■

We now introduce the open set Ω defined by

$$\Omega = \{ \ (T, Y, c) \in \mathcal{O}, \ \|(T, Y)\|_{C^1[0,a]} < \beta, \ \alpha < T < \beta, \ \alpha < c < \beta \ \}, \tag{6.7}$$

where α and β are positive constants.

Theorem 6.3. *There exists constants α and β such that for all $\tau \in [0,1]$ and $a \geq 1$, the Leray-Schauder degree $d(I - \mathcal{K}_\tau, \Omega, 0)$ is well defined.*

In order to establish this theorem, we have to show that for α small enough and β large enough we have

$$\forall \tau \in [0,1], \qquad 0 \notin (I - \mathcal{K}_\tau)(\partial\Omega). \tag{6.8}$$

This will be obtained in the next section by estimating fixed points of $\mathcal{K}_\tau$.

6.3. Existence of the degree

We estimate in this Section the fixed points (T, Y, c) of $\mathcal{K}_\tau$ for $\tau \in [0,1]$. By definition, we have $T > 0$, $c > 0$, and $(T, Y, c) = (t, y, c + t(0) - T^{\mathrm{i}})$, so that the equations obtained from (6.5) with $t = T$ and $y = Y$ hold and $T(0) = T^{\mathrm{i}}$. A priori estimates are successively obtained in the following lemmas.

Lemma 6.4. *Let (T, Y, c) be a fixed point of $\mathcal{K}_\tau$. Then the mass fractions are positive $Y > 0$ and sum up to unity $\langle U, Y \rangle = 1$.*

Proof. We first deduce from the species equations (6.5) that $c\langle U, Y\rangle' = 0$ since we have $R(\mathcal{L}^\sharp) = \mathcal{U}^\perp$. As a consequence, $\langle U, Y \rangle$ is a constant which is unity from (6.6), and this shows that $\widetilde{Y} = Y^+$

Step 1. We first establish that $Y(0) \geq 0$. Arguing by contradiction, assume that there exists $k \in S$ such that $Y_k(0) < 0$. Then from the species equations written at $x = 0$ we have $c(Y_k(0) - \xi_k^{\mathrm{f}}) - \sum_{l \in S} \mathcal{L}_{kl}\big((T(0), Y^+(0)\big)Y_l'(0) = 0$, and we also have $Y_k^+(0) = 0$, so that from Lemma 4.10 we deduce that

$$Y_k'(0) = \frac{c}{d_k(0)}(Y_k(0) - Y_k^{\mathrm{f}}) < 0.$$

Then Y_k is negative over an interval of the form $(0,\epsilon)$ with $\epsilon > 0$. Over this interval $(0,\epsilon)$ we now have

$$d_k Y_k' = c(Y_k - Y_k^{\mathrm{f}}) - \tau \int_0^x m_k \widetilde{\mathcal{P}}_k \, du,$$

since $\widetilde{\omega}_k = \widetilde{\mathcal{P}}_k$, for $\widetilde{Y}_k = Y_k^+ = 0$. This shows that Y_k' is negative and Y_k is decreasing. By using a forward shooting argument, we deduce that Y_k remains negative, contradicting the backward initial condition $Y_k(a) = Y_k^{\mathrm{e}} > 0$.

Step 2. We now claim that $Y \geq 0$. Aguing by contradiction, assume that there exists a point x_1 and a species $k \in S$ such that $Y_k(x_1) < 0$. From the preceding discussion and since $Y(a) = Y^{\mathrm{e}}$, we necessarily have $x_1 \in (0,a)$. Define now

$$x_0 = \sup\{\, t \in (0,x_1],\ Y_k(t) = 0 \,\}.$$

This set is nonempty since $Y_k(0) \geq 0$ and $Y_k(x_1) < 0$. In addition, x_0 is different from x_1 since Y_k is Lipchitzian. Indeed, we have $|Y_k(x_1)| \leq M(x_1 - t)$ for any $t < x_1$ such that $Y_k(t) = 0$ where M is a Lipchitz constant for Y_k. Since $x_0 \neq x_1$, we now consider the interval (x_0,x_1) where Y_k is negative since $Y_k(x_1) < 0$ and Y_k cannot change of sign over (x_0,x_1) by construction. There exists $\bar{x} \in (x_0,x_1)$ with $Y_k'(\bar{x}) < 0$ and a forward shooting argument now shows that Y_k' and Y_k are negative over $[\bar{x},a]$, an obvious contradiction with $Y_k(a) = Y_k^{\mathrm{e}}$.

Step 3. We now show that $Y(0) > 0$. Arguing by contradiction, assume that $Y_k(0) = 0$ for some $k \in S$. Then from the species equation, we obtain that

$$Y_k'(0) = \frac{c}{d_k(0)}(Y_k(0) - Y_k^{\mathrm{f}}) \leq 0,$$

and since $Y \geq 0$, we cannot have $Y_k'(0) < 0$ so that necessarily $Y_k^{\mathrm{f}} = 0$. From the preceding steps, we know that $\langle Y, U\rangle = 1$ and that $Y \geq 0$, so that $\widetilde{Y} = Y$ and from (6.5) the solution is twice differentiable. Deriving the species relations and substituting $x = 0$ we deduce that

$$d_k(0) Y_k''(0) = -\tau m_k \mathcal{P}_k(0) \leq 0.$$

Since $Y \geq 0$, $Y_k''(0)$ cannot be negative so that necessarily $\mathcal{P}_k(0) = 0$. We now introduce the set $\mathcal{I} = \{\, k \in S,\ Y_k(0) = 0 \,\}$ and from the preceding discussion we have

$$\forall k \in \mathcal{I},\ Y_k(0) = 0,\ Y_k'(0) = 0,\ Y_k''(0) = 0,\ \tau\mathcal{P}_k(0) = 0. \tag{6.9}$$

Now if $\tau > 0$, any reaction creating a species $\mathcal{S}_k$, with $k \in \mathcal{I}$, needs at least one species $\mathcal{S}_i$ with $i \in \mathcal{I}$ as a reactant, otherwise one would get a positive production term. This shows that the mass fractions Y_k, $k \in \mathcal{I}$, are factorized in the production terms ω_l, $l \in \mathcal{I}$. Now the mass fractions Y_k, $k \in \mathcal{I}$, are solution of the system

$$cY_k' = \Big(d_k(x) Y_k' + Y_k \pi_k(x)\Big)' + \tau m_k \omega_k,$$

where d_k and π_k are defined in Lemma 4.10. However, this system has a locally unique solution from the Cauchy-Lipchitz theorem, but also admits the trivial solution.

A shooting argument now shows that $Y_k = 0$ over $[0, a]$ for any $k \in \mathcal{I}$, an obvious contradiction.

Step 4. We finally establish that $Y > 0$. Still arguing by contradiction, we consider the first point x_0 such that there exists $l \in [1, n]$ with $Y_l(x_0) = 0$. Of course we have $x_0 \neq a$ since $Y_l^{\mathrm{e}} > 0$. At this point, since $Y_l > 0$ on $[0, x_0)$, we have $Y_l'(x_0) \leq 0$. We cannot have $Y_l'(x_0) < 0$ since $Y \geq 0$ so that $Y_l'(x_0) = 0$ and $Y_l(x_0) = 0$. We can now proceed as in the preceding step to conclude that Y_l is locally zero which contradicts the definition of x_0 and the proof is complete. ∎

Lemma 6.5. *Let (T, Y, c) be a fixed point of $\mathcal{K}_\tau$ and assume that is has been extended over $(-\infty, 0)$ by using Proposition 5.3. We know from Lemma 6.4 and Proposition 5.3 that the species are positive so that the entropy and the dissipation rate are well defined. We then have the entropic estimates*

$$\int_{-\infty}^{a} \kappa \, dx = c(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}}), \tag{6.10}$$

where

$$\kappa = \lambda\Big(\frac{T'}{T}\Big)^2 + \frac{p}{T} \sum_{k,l \in S} D_{kl}\big(\gamma_k' + \chi_k(T'/T)\big)\,\big(\gamma_l' + \chi_l(T'/T)\big) - \tau \sum_{k \in S} \frac{g_k m_k \omega_k}{T}, \tag{6.11}$$

and where we use the notation $\omega(x) = 0$ for $x < 0$.

Proof. Since the species are positive and we may thus use the entropy governing equation

$$c\,\sigma' + \langle \partial_\xi \sigma, \phi \rangle' = \kappa,$$

where the dissipation rates κ is given by (6.11). We also know from Proposition 5.3 that the integral of κ over $(-\infty, 0)$ is given by (5.3). Integrating the entropy conservation equation over $[0, a]$ thus yields

$$c(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}}) + \big\langle (\partial_\xi \sigma)^{\mathrm{e}}, \phi(a) \big\rangle = \int_{-\infty}^{a} \kappa \, dx, \tag{6.12}$$

where $(\partial_\xi \sigma)^{\mathrm{e}} = (\partial_\xi \sigma)(\xi^{\mathrm{e}})$.

On the other hand, we know that $(\partial_Y \sigma)^{\mathrm{e}} \in (M\mathcal{R})^\perp$ so that $(\partial_\xi \sigma)^{\mathrm{e}} \in (0, M\mathcal{R})^\perp$. Multiplying the species conservation equations by $(\partial_\xi \sigma)^{\mathrm{e}}$ and integrating over $(-\infty, a]$ then yields

$$c\big\langle (\partial_\xi \sigma)^{\mathrm{e}}, \xi^{\mathrm{e}} - \xi^{\mathrm{f}} \big\rangle + \big\langle (\partial_\xi \sigma)^{\mathrm{e}}, \phi(a) \big\rangle = 0.$$

However, $\xi^{\mathrm{e}} - \xi^{\mathrm{f}} \in (0, M\mathcal{R})^\perp$ since $Y^{\mathrm{e}} - Y^{\mathrm{f}} \in M\mathcal{R}$ from element conservation and since $h^{\mathrm{e}} = h^{\mathrm{f}}$. As a consequence, we have $\big\langle (\partial_\xi \sigma)^{\mathrm{e}}, \xi^{\mathrm{e}} - \xi^{\mathrm{f}} \big\rangle = 0$ and $\big\langle (\partial_\xi \sigma)^{\mathrm{e}}, \phi(a) \big\rangle = 0$ and the proof is complete from (6.12). ∎

Lemma 6.6. *Let (T, Y, c) be a fixed point of $\mathcal{K}_\tau$. Then there exists positive constants α and β independent of a such that $\alpha < T < \beta$.*

Proof. We start from the entropy conservation equation

$$c\,\sigma' + \langle \partial_\xi \sigma, \phi \rangle' = \kappa,$$

that we multiply by $\langle \partial_\xi \sigma, \phi \rangle$ and integrate over $[0,x]$. This yields the identity

$$\tfrac{1}{2}\langle \partial_\xi \sigma, \phi \rangle^2 = \tfrac{1}{2}\langle \partial_\xi \sigma, \phi \rangle^2(0) + \int_0^x \Big(\kappa \, \langle \partial_\xi \sigma, \phi \rangle - c\sigma' \langle \partial_\xi \sigma, \phi \rangle \Big)\, du.$$

The first integral term can be bounded by

$$\int_0^x \kappa \, \langle \partial_\xi \sigma, \phi \rangle \, du \;\le\; \int_0^x \big(c + \frac{1}{c} \langle \partial_\xi \sigma, \phi \rangle^2 \big) \kappa \, du \;\le\; bc^2 + \frac{1}{c} \int_0^x \langle \partial_\xi \sigma, \phi \rangle^2 \kappa \, du.$$

On the other hand, the second integral term can be estimated with

$$\big| \sigma' \langle \partial_\xi \sigma, \phi \rangle \big| = \Big| c_p \frac{T'}{T} + \sum_{k\in S} s_k Y_k' \Big| \; \Big| -\lambda \frac{T'}{T} + \sum_{k\in S} s_k \mathcal{F}_k \Big|,$$

which yields, by using the definition of the species entropies s_k, $k \in S$, that

$$\begin{aligned} \big| \sigma' \langle \partial_\xi \sigma, \phi \rangle \big| \;\le\; & \; b \, \varphi(T)^{1/2} \Big(\big| \frac{T'}{T} \big| + \sum_{k\in S} \big(1 + |\log Y_k| + |\log T| \big) |Y_k'| \Big) \\ & \varphi(T)^{-1/2} \Big(\lambda \big| \frac{T'}{T} \big| + \sum_{k\in S} \big(1 + |\log Y_k| + |\log T| \big) |\mathcal{F}_k| \Big). \end{aligned}$$

We now use the entropic estimates (6.10) and Schwartz inequality in order to estimate the integral of $\big|\sigma' \langle \partial_\xi \sigma, \phi \rangle\big|$. By using $Y_k |\log Y_k|^2 \le 1$ for $0 < Y_k \le 1$ and the expressions (4.10) for the multicomponent fluxes, we deduce that

$$\int_0^x \big| \sigma' \langle \partial_\xi \sigma, \phi \rangle \big| \, du \;\le\; b\Big(c + \int_0^x |\log T|^2 \, \kappa \, du \Big).$$

On the other hand, by integrating the entropy conservation equation over $[0,x]$, we have

$$c(\sigma - \sigma^{\mathrm{f}}) + \langle \partial_\xi \sigma, \phi \rangle = \int_{-\infty}^x \kappa \, du,$$

which implies that

$$c\,|\log T| \;\le\; bc + \big| \langle \partial_\xi \sigma, \phi \rangle \big|. \tag{6.13}$$

since the specific heats are bounded by positive constants. Combining these results yields that

$$\int_0^x \big| \sigma' \langle \partial_\xi \sigma, \phi \rangle \big| \, du \;\le\; bc + \frac{b}{c^2} \int_0^x \langle \partial_\xi \sigma, \phi \rangle^2 \kappa \, du,$$

so that

$$\langle \partial_\xi \sigma, \phi \rangle^2 \;\le\; bc^2 + \frac{b}{c} \int_0^x \langle \partial_\xi \sigma, \phi \rangle^2 \, \kappa \, du.$$

From Gronwald Lemma, we obtain

$$\langle \partial_\xi \sigma, \phi \rangle^2 \leq bc^2,$$

and using (6.13) we conclude that

$$|\log T| \leq b,$$

and the proof is complete. ∎

It is the first time that an upper bound for the temperature is obtained in a flame with nontrivial transport. Note also that the natural entropy production weighted norm has been used in the proof of Lemma 6.6.

We now estimate the eigenvalue c of the flame problem. In the following lemma, we obtain an upper bound independent of a and a lower bound which depends on a. The existence of a lower bound independent of a will only be needed when passing to the limit $a \to \infty$ and is postponed to Section 7.

Lemma 6.7. *Let (T, Y, c) be a fixed point of $\mathcal{K}_\tau$ and assume that $a \geq 1$. Then there exists positive constants α and β such that $\alpha < c < \beta$ and β is independent of a.*

Proof. When thermal diffusion is not included, there exists a simple way to get an upper bound for c. Indeed, using the identity $c(\xi - \xi^{\mathrm{f}}) + \phi = \tau \int_0^x w du$, we have

$$c \sum_{k \in S} Y_k^{\mathrm{f}} (h_k - h_k^{\mathrm{f}}) - \lambda T' = \tau \sum_{k \in S} h_k \int_0^x m_k \omega_k du.$$

Assume now that $a \geq 1$, and denote by b_0 an upper bound—independent of a—of the sum in the right member for $x \in [0,1]$. Then either $c\, \underline{c}_p (T^{\mathrm{i}} - T^{\mathrm{f}}) \leq b_0$, and there is nothing to prove, or $c\, \underline{c}_p (T^{\mathrm{i}} - T^{\mathrm{f}}) \geq b_0$ and a shooting argument shows that $T \geq T^{\mathrm{i}}$ over $[0,1]$. In this situation, and we may write the above equality at a point $x \in [0,1]$ such that $T'(x) = T(1) - T(0)$ to obtain an upper bound for c.

When thermal diffusion is included, we first note that for $x \geq 0$

$$c(\sigma - \sigma^{\mathrm{f}}) + \langle \partial_\xi \sigma, \phi \rangle = \int_{-\infty}^x \kappa \, du \geq \int_0^x \kappa \, du = c\Big(\sigma(0) - \sigma^{\mathrm{f}} - \big\langle \partial_\xi \sigma(0), \xi(0) - \xi^{\mathrm{f}} \big\rangle \Big).$$

Since $T(0) = T^{\mathrm{i}} > T^{\mathrm{f}}$, we deduce that there exists $\delta > 0$ such that for any $x \geq 0$

$$\sigma - \sigma^{\mathrm{f}} + \frac{1}{c} \langle \partial_\xi \sigma, \phi \rangle \geq \delta > 0.$$

In addition, we have $\langle \phi, \phi \rangle \leq b\kappa$ and $\langle \partial_\xi \sigma, \phi \rangle^2 \leq b\kappa$ since the temperature is uniformly bounded and since $(\log \gamma)^2 \gamma \leq 1$ for $\gamma \leq 1$. As a consequence, we have

$$\int_0^1 \big(\langle \phi, \phi \rangle + \langle \partial_\xi \sigma, \phi \rangle^2 \big) \, dx \; \leq \; bc$$

and from the governing equations $c(\xi - \xi^{\mathrm{f}}) + \phi = \int_0^x w du$ we finally obtain

$$\int_0^1 \Big(\big\| \xi - \xi^{\mathrm{f}} - \frac{\tau}{c} \int_0^x w \, du \big\|^2 + \big| \frac{1}{c} \langle \partial_\xi \sigma, \phi \rangle \big|^2 \Big) \, dx \; \le \; bc.$$

We now use the uniform continuity of σ over the compact set $Y \ge 0$, $\langle Y, U \rangle = 1$, and $\mathfrak{a} \le T \le \mathfrak{b}$. More specifically, there exists η such that $\|\xi_1 - \xi_0\| < \eta$ implies that $\|\sigma(\xi_1) - \sigma(\xi_0)\| < \delta/2$.

Now for $x \in (0,1)$ we have the following alternative. Either $\|\xi - \xi^{\mathrm{f}}\| < \eta$ and then $\|\sigma(\xi) - \sigma(\xi^{\mathrm{f}})\| < \delta/2$ and the entropic estimates yields

$$\big| \frac{1}{c} \langle \partial_\xi \sigma, \phi \rangle \big| \ge \delta/2.$$

Or we have $\|\xi - \xi^{\mathrm{f}}\| \ge \eta$ so that for

$$\frac{\beta_w}{c} \le \tfrac{1}{2}\eta,$$

where β_w is a uniform bound of $\| \int_0^1 w \, dx\|$, we then have

$$\|\xi - \xi^{\mathrm{f}} - \frac{\tau}{c} \int_0^x w \, du\| \ge \tfrac{1}{2}\eta.$$

We have thus shown that $c \ge 2\beta_w/\eta$ implies that

$$c \, \tfrac{1}{4} \inf \Big(\eta^2, \delta^2 \Big) \le b,$$

so that c is bounded from above.

For the lower bound, we remark that

$$|T(a) - T(0)| \; \le \; \int_0^a |T'(x)| \, dx \; \le \; \sqrt{a} \int_0^a |T'(x)|^2 \, dx,$$

and we also have $|T'|^2 \le b\kappa$ uniformy from the temperature bounds. As a consequence, we obtain that

$$T^{\mathrm{e}} - T^{\mathrm{i}} \; \le \; b\sqrt{a} \int_0^a \kappa \, dx \; \le \; bc\sqrt{a},$$

and this yields a lower bound for c which depends on a. ∎

We now estimate the derivatives of fixed points of $\mathcal{K}_\tau$.

Lemma 6.8. *Let (T, Y, c) be a fixed point of $\mathcal{K}_\tau$ and assume that $a \ge 1$. Then there exists a positive constant β independent of a such that $\|(T,Y)\|_{C^3[0,a]} < \beta$ and such that $\|(T', Y')\|_{H^2[0,a]} < \beta$*

Proof. We use the variable ξ for convenience and from the entropic estimate and the upper bounds derived in the previous lemmas we obtain that

$$\int_{-\infty}^a \|\xi'\|^2 \, dx \; \le \; \beta. \tag{6.14}$$

On the other hand, we may use the expression (3.31) of the dissipation rate

$$\zeta = \sum_{i\in R} \widehat{K}_i\big(\langle M\nu_i^{\rm d}, \mu\rangle - \langle M\nu_i^{\rm r}, \mu\rangle\big)\ \big(\exp\langle M\nu_i^{\rm d}, \mu\rangle - \exp\langle M\nu_i^{\rm r}, \mu\rangle\big).$$

Since $\gamma_k \leq 1$, $k \in S$, we know from (2.20) that $\langle \mu, M\nu_i^{\rm d}\rangle$ and $\langle \mu, M\nu_i^{\rm r}\rangle$ are bounded from above. As a consequence, there exists b such that

$$\big|\exp\langle \mu, M\nu_i^{\rm d}\rangle - \exp\langle \mu, M\nu_i^{\rm r}\rangle\big| \ \leq\ b\big|\langle \mu, M\nu_i^{\rm d}\rangle - \langle \mu, M\nu_i^{\rm r}\rangle\big|,$$

and, using now the positivity of $\widehat{K}_i$, $i \in R$, and the uniform estimates for the temperature, we conclude that

$$\sum_{i\in R} r_i^2 \ \leq\ b\zeta,$$

so that finally, using the entropic estimates, there exists b such that

$$\tau \int_0^a \|w\|^2\, dx \leq b.$$

From the governing equations $c\xi' + \phi' = \tau w$, where $w = 0$ for $x < 0$, and from $0 \leq \tau \leq 1$, we now deduce that

$$\int_{-\infty}^a \|\phi'\|^2\, dx \leq \beta,$$

and from Sobolev injection applied to $\phi = -\mathcal{L}\xi'$ we obtain that $\|\phi\| \leq \beta$ uniformly over $(-\infty, a]$ and from $\xi' = -\mathcal{L}^\sharp\phi$ we further obtain that $\|\xi'\| \leq \beta$ uniformly over $(-\infty, a]$. Finally, from the governing equations, we deduce that $\|\phi'\|$ is uniformly bounded and upon expanding the derivatives we conclude that $\|\xi''\|$ is also uniformly bounded. The L^∞ estimates for ϕ'' and ξ''' and the $H^2[0, a]$ estimates of derivatives are similar. ∎

6.4. Calculation of the degree

From the homotopy invariance of the degree, we have

$$d(I - \mathcal{K}_1, \Omega, 0) = d(I - \mathcal{K}_0, \Omega, 0), \tag{6.15}$$

and the map $\mathcal{K}_0$ no longer involves chemistry source terms. In order to evaluate this degree, we need a second homotopy in order to simplify transport properties and thermodynamics.

We introduce the operator

$$\mathcal{H}_\tau \ :\ \mathcal{O} \longrightarrow \mathcal{B},$$

defined by

$$\mathcal{H}_\tau(T, Y, c) = \Big(t, y, c + t(0) - T^{\rm i}\Big), \tag{6.16}$$

where (t, y) are solutions of the system

$$\Big(\widetilde{c}_p^{\tau}\, t' + \sum_{k\in S} h_k^{\tau}\, y_k',\, y'\Big)^{\star} = (\widetilde{\mathcal{L}}^{\tau})^{\sharp}\bigg(c\Big(\int_0^t \widetilde{c}_p^{\tau}\, dx + \sum_{k\in S} h_k^0 y_k,\, y\Big)^{\star} - c\,\xi^{\mathrm{f},\tau}\bigg), \tag{6.17}$$

with the initial conditions

$$t(a) = T^{\mathrm{e}}, \qquad y(a) = Y^{\mathrm{e}}. \tag{6.18}$$

In these expressions, we have used the notation

$$\widetilde{c}_{pk}^{\tau} = \tau \widetilde{c}_{pk} + (1-\tau)\overline{c}_p,$$

$$\widetilde{\lambda}^{\tau} = \tau\widetilde{\lambda} + (1-\tau)\overline{\lambda},$$

$$\widetilde{\mathcal{C}}^{\tau} = \tau\widetilde{\mathcal{C}} + (1-\tau)\overline{D}\Big(I\langle Y, U\rangle - Y\otimes U\Big),$$

$$\widetilde{\chi}_k^{\tau} = \tau\widetilde{\chi}_k,$$

$$m_k^{\tau} = \tau m_k + (1-\tau) m_0,$$

$$\xi^{\mathrm{f},\tau} = \Big(\sum_{k\in S} Y_k^{\mathrm{f}}\,(h_k^0 + \int_0^{T^{\mathrm{f}}} \widetilde{c}_{pk}^{\tau} dx),\, Y^{\mathrm{f}}\Big)^{\star},$$

where $\overline{c}_p$, $\overline{\lambda}$, $\overline{D}$, and m_0 are fixed positive constants such that

$$\frac{\overline{\lambda}}{\overline{c}_p\overline{D}} = 1,$$

and where $\widetilde{\mathcal{L}}^{\tau}$ is taken as in Definition 4.8 in terms of $\widetilde{\mathcal{C}}^{\tau}$, $\widetilde{\chi}^{\tau}$, $\widetilde{\lambda}^{\tau}$, $\widetilde{c}_p^{\tau}$, and m^{τ}.

The idea behind this new homotopy is to obtain trivial thermodynamics and trivial transport fluxes for $\tau = 0$. One could also simultaneously modify the chemistry source terms, thermodynamic properties and transport properties in a single homotopy. However, it requires changing the equilibrium temperature boundary condition—which depends on thermodynamics—and simultaneously to change the cold temperature boundary conditions, in order to prevent any temperature crossings associated with modified equilibrium temperatures. Using two distinct homotopies somewhat simplifies the presentation.

Proposition 6.9. *The operator $\mathcal{H}_\tau : \mathcal{O} \to \mathcal{B}$ is well posed and the degree $d(I-\mathcal{H}_\tau, \Omega, 0)$ is well defined for $\tau \in [0,1]$ and $a \geq 1$. Moreover, for any closed bounded set B in $\mathcal{O}$, the map $\mathcal{H} : [0,1]\times B \to \mathcal{B}$ defined by $\mathcal{H}\big(\tau, (T, Y, c)\big) = \mathcal{H}_\tau(T, Y, c)$, is compact.*

Proof. It is exactly similar to the preceding case up to minor modifications. For instance, the entropic estimates now reads

$$\int_{-\infty}^{a} \kappa\, dx = c\Big(\sigma(\xi^{\mathrm{e},\tau}) - \sigma(\xi^{\mathrm{f},\tau}) - \big\langle \partial_\xi\sigma(\xi^{\mathrm{e},\tau}), \xi^{\mathrm{e},\tau} - \xi^{\mathrm{f},\tau}\big\rangle\Big),$$

where

$$\xi^{\mathrm{e},\tau} = \Big(\sum_{k \in S} Y_k^{\mathrm{e}} \big(h_k^0 + \int_0^{T^{\mathrm{e}}} \widetilde{c}_{pk}^{\tau} dx \big),\, Y^{\mathrm{e}} \Big)^{\star},$$

since $\xi^{\mathrm{e},\tau}$ does not anymore coincide with the maximum of σ on the conservation simplex, the specific heats being modified along the homotopy path. ■

From the homotopy invariance of the degree, we now obtain that

$$d(I - \mathcal{K}_1, \Omega, 0) = d(I - \mathcal{H}_0, \Omega, 0), \tag{6.19}$$

and a straightforward calculation—making use of $\langle y', U \rangle = 0$—yields that the map $\mathcal{H}_0$ has the simple structure

$$\mathcal{H}_0(T, Y, c) = \Big(t_c, y_c, c + t_c(0) - T^{\mathrm{i}} \Big), \tag{6.20}$$

where t_c and y_c are given by

$$t_c(x) = T^{\mathrm{f}} + (T^{\mathrm{e}} - T^{\mathrm{f}}) \exp(c\,(x-a)\overline{c}_p/\overline{\lambda}), \tag{6.21}$$

$$y_c(x) = Y^{\mathrm{f}} + (Y^{\mathrm{e}} - Y^{\mathrm{f}}) \exp(c\,(x-a)\overline{c}_p/\overline{\lambda}), \tag{6.22}$$

and only depend on c.

We can then define a third homotopy by introducing the operator

$$\mathcal{A}_\tau \;:\; \mathcal{O} \longrightarrow \mathcal{B},$$

defined by

$$\mathcal{A}_\tau(T, Y, c) = \Big(\tau t_c, \tau y_c, c + t_c(0) - T^{\mathrm{i}} \Big).$$

One may easily check that $\mathcal{A}_\tau$ is well posed and that the degree $d(I - \mathcal{A}_\tau, \Omega, 0)$ is well defined. We thus obtain that

$$d(I - \mathcal{K}_1, \Omega, 0) = d(I - \mathcal{A}_0, \Omega, 0),$$

so that from

$$\mathcal{A}_0(T, Y, c) = \Big(0, 0, c + t_c(0) - T^{\mathrm{i}} \Big)$$

and the multiplicative properties of the degree, we have

$$d(I - \mathcal{K}_1, \Omega, 0) = d(T^{\mathrm{i}} - t_c(0), (\alpha, \beta), 0).$$

From (6.21) we have

$$t_c(0) = T^{\mathrm{f}} + (T^{\mathrm{e}} - T^{\mathrm{f}}) \exp(-c\, a\overline{c}_p/\overline{\lambda}),$$

so that finally

$$d(I - \mathcal{K}_1, \Omega, 0) = 1,$$

since $\alpha < T^{\rm f} < T^{\rm i} < T^{\rm e} < \beta$ and there exists a solution to the problem posed on a bounded domain.

7. EXISTENCE OF SOLUTIONS

In this section, we pass to the limit $a \to \infty$ and obtain a solution of the anchored flame problem. A first step is to derive a lower bound for the flame eigenvalue c which is independent of a. Another important point is to investigate the behavior of the solution near the equilibrium state $\xi^{\rm e}$.

7.1. Uniform estimates for c

Lemma 7.1. *For $0 < \delta < \sigma^{\rm e} - \sigma^{\rm f}$ there exists a unique point x_δ such that*

$$\int_{x_\delta}^{a} \kappa \, dx = \delta c.$$

Proof. The function Ψ defined on $(-\infty, a]$ by

$$\Psi(x) = \int_{-\infty}^{x} \kappa \, du,$$

is strictly increasing since κ is strictly positive over $(-\infty, a]$. Arguing by contradiction, we indeed note that for $x_0 < 0$, $\kappa(x_0) = 0$ implies that $\phi(x_0) = 0$ and thus that $\xi(x_0) = \xi^{\rm f}$ from (5.2) and the Cauchy-Lipchitz theorem yields $\xi(x) = \xi^{\rm f}$ for any $x \le 0$, contradicting $T^{\rm f} \ne T^{\rm i}$. Similarly, for $x_0 \ge 0$, $\kappa(x_0) = 0$ implies that $\xi'(x_0) = 0$ and $\zeta(x_0) = 0$. Since $Y(x_0) > 0$, we deduce from $\zeta(x_0) = 0$ that $\xi(x_0)$ is an equilibrium point and from the Cauchy-Lipchitz theorem we obtain that $\xi(x) = \xi(x_0)$ for $0 \le x \le a$, contradicting $T(0) = T^{\rm i} \ne T^{\rm e} = T(a)$. ∎

We now show that $\xi(x)$ is close to $\xi^{\rm e}$ when the integral of the dissipation rate κ over the interval $[x, a]$ is small, in particular for $x \in [x_\delta, a]$.

Lemma 7.2. *There exists a constant β_0 such that for any $a \ge 1$ we have*

$$\forall x \in [0, a], \qquad \big\|\xi(x) - \xi^{\rm e}\big\|^2 \;\le\; \beta_0 \Big(\frac{1}{c}\int_x^a \kappa(u)\, du\Big)^{1/2}. \tag{7.1}$$

Proof. We first note that there exists α such that we have uniformly

$$\|\xi - \xi^{\rm e}\|^2 \;\le\; \beta\Big(\sigma^{\rm e} - \sigma - \big\langle (\partial_\xi \sigma)^{\rm e}, \xi^{\rm e} - \xi \big\rangle\Big),$$

since T is uniformly bounded and $\langle Y, U\rangle = 1$. Since $(\partial_\xi \sigma)^{\rm e} \in (0, M\mathcal{R})^\perp$ we easily obtain, by combining the conservation equations and the entropy equation, that

$$c\Big(\sigma' - \big\langle (\partial_\xi \sigma)^{\rm e}, \xi \big\rangle'\Big) + \Big(\big\langle \partial_\xi \sigma, \phi \big\rangle - \big\langle (\partial_\xi \sigma)^{\rm e}, \phi \big\rangle\Big)' = \kappa. \tag{7.2}$$

We multiply this equation by $\psi = \big\langle \partial_\xi \sigma, \phi \big\rangle - \big\langle (\partial_\xi \sigma)^{\rm e}, \phi \big\rangle$ and integrate over $[x,a]$. This yields

$$-\tfrac{1}{2}\psi^2 = \int_x^a \kappa \psi \, du - c \int_x^a \big(\sigma' - \langle (\partial_\xi \sigma)^{\rm e}, \xi' \rangle\big)\, \psi \, du.$$

However, we can now estimate

$$\int_x^a \big|\sigma' - \langle (\partial_\xi \sigma)^{\rm e}, \xi' \rangle\big|\, |\psi| \, du, \ \le \ \beta \int_x^a \kappa \, du,$$

so that by using $|\psi| \le c + (1/c)\psi^2$ we obtain

$$\psi^2 \ \le \ \beta c \int_x^a \kappa \, du + \frac{\beta}{c} \int_x^a \psi^2 \, \kappa \, du.$$

Using a (backward) generalized Gronwald Lemma [Bou76] we now obtain

$$\psi^2 = \Big| \big\langle \partial_\xi \sigma, \phi \big\rangle - \big\langle (\partial_\xi \sigma)^{\rm e}, \phi \big\rangle \Big|^2 \ \le \ \beta c \int_x^a \kappa \, du.$$

On the other hand, by integrating (7.2) over $[x,a]$, we get

$$c \Big(\sigma^{\rm e} - \sigma - \big\langle (\partial_\xi \sigma)^{\rm e}, \xi^{\rm e} - \xi \big\rangle \Big) - \psi = \int_x^a \kappa(u) \, du,$$

which yields that

$$\sigma^{\rm e} - \sigma - \big\langle (\partial_\xi \sigma)^{\rm e}, \xi^{\rm e} - \xi \big\rangle \ \le \ \beta \Big(\frac{1}{c} \int_x^a \kappa(u) \, du \Big)^{1/2},$$

which completes the proof. ■

We now estimate more closely the integral of the dissipation rate κ when ξ is close to $\xi^{\rm e}$. This result will then be applied over the interval $[x_\delta, a]$.

Proposition 7.3. *There exists positive constants $\epsilon_1 < T^{\rm e} - T^{\rm f}$ and β_1 such that for any $a \ge 1$*

$$\forall x \in (-\infty, a], \qquad \|\xi(x) - \xi^{\rm e}\| < \epsilon_1 \quad \Longrightarrow \quad \int_x^a \kappa(u) \, du \ \le \ \beta_1 \kappa(x).$$

Proof. We define $\mathfrak{v}^{\rm e}$ as the unique equilibrium point in the conservation maniflod $\xi + (0, M\mathcal{R})$. By construction, we have $(\partial_\xi \sigma)(\mathfrak{v}^{\rm e}) \in (0, M\mathcal{R})^\perp$ and by combining the conservation equations and the entropy equation we easily obtain that

$$c\Big(\sigma^{\rm e} - \sigma - \big\langle (\partial_\xi \sigma)(\mathfrak{v}^{\rm e}), \xi^{\rm e} - \xi \big\rangle \Big) + \Big\langle (\partial_\xi \sigma)(\mathfrak{v}^{\rm e}) - (\partial_\xi \sigma), \phi \Big\rangle = \int_x^a \kappa(u) \, du.$$

We can rewrite this identity in the form

$$c\Big(\sigma(\mathfrak{v}^{\mathrm{e}}) - \sigma - \langle(\partial_\xi\sigma)(\mathfrak{v}^{\mathrm{e}}), \mathfrak{v}^{\mathrm{e}} - \xi\rangle\Big) + c\Big(\sigma^{\mathrm{e}} - \sigma(\mathfrak{v}^{\mathrm{e}}) - \langle(\partial_\xi\sigma)(\mathfrak{v}^{\mathrm{e}}), \xi^{\mathrm{e}} - \mathfrak{v}^{\mathrm{e}}\rangle\Big) \\ + \Big\langle(\partial_\xi\sigma)(\mathfrak{v}^{\mathrm{e}}) - (\partial_\xi\sigma), \phi\Big\rangle = \int_x^a \kappa(u)\,du, \tag{7.3}$$

so that by using $(\partial_\xi\sigma)(\mathfrak{v}^{\mathrm{e}}) \in (0, M\mathcal{R})^\perp$ and $\xi - \mathfrak{v}^{\mathrm{e}} \in (0, M\mathcal{R})$, and taking into account the concavity of σ, we obtain

$$c\,\big(\sigma(\mathfrak{v}^{\mathrm{e}}) - \sigma\big) + \Big\langle(\partial_\xi\sigma)(\mathfrak{v}^{\mathrm{e}}) - (\partial_\xi\sigma), \phi\Big\rangle \;\geq\; \int_x^a \kappa(u)\,du. \tag{7.4}$$

On the other hand, when ξ is close enough to ξ^{e}, say $\|\xi(x) - \xi^{\mathrm{e}}\| < \epsilon_1$, we can write that

$$\alpha\|\mathfrak{v}^{\mathrm{e}} - \xi\|^2 \;\leq\; \sigma(\mathfrak{v}^{\mathrm{e}}) - \sigma(\xi) \;\leq\; \beta\|\mathfrak{v}^{\mathrm{e}} - \xi\|^2,$$

and

$$\Big|\langle\partial_\xi\sigma(\mathfrak{v}^{\mathrm{e}}) - \partial_\xi\sigma, \phi\rangle\Big| \;\leq\; \beta\Big(\|\mathfrak{v}^{\mathrm{e}} - \xi\|^2 + \|\phi\|^2\Big),$$

so that

$$\Big|\langle\partial_\xi\sigma(\mathfrak{v}^{\mathrm{e}}) - \partial_\xi\sigma, \phi\rangle\Big| \;\leq\; \beta\Big(\sigma(\mathfrak{v}^{\mathrm{e}}) - \sigma(\xi) + \langle(\partial_\xi^2\sigma)\xi', \phi\rangle\Big).$$

Finally, using the local stability inequality of Proposition 3.11, we deduce that there exists β_1 such that

$$\int_x^a \kappa(u)\,du \;\leq\; \beta_1\kappa(x),$$

for $\|\xi(x) - \xi^{\mathrm{e}}\| < \epsilon_1$ since c is bounded by above independently of a for $a \geq 1$ and the proof is complete. ∎

By using Proposition 7.3, we now obtain that the exponential decay of the integral of the dissipation rate κ near equilibrium.

Corrolary 7.4. *Let ϵ such that $0 < \epsilon < T^{\mathrm{e}} - T^{\mathrm{i}}$ and define $z_\epsilon \geq 0$ to be the largest x such that $\|\xi(x) - \xi^{\mathrm{e}}\| = \epsilon$ and $\|\xi(t) - \xi^{\mathrm{e}}\| \leq \epsilon$ for all $t \in [x, a]$. Then there exists a constant $\mathfrak{d}$ such that for any $a \geq 1$*

$$\forall \epsilon \in (0, \epsilon_1], \quad \forall x \in [z_\epsilon, a], \qquad \int_x^a \kappa(u)\,du \;\leq\; \Big(\int_{z_\epsilon}^a \kappa(u)\,du\Big)\exp\big(-\mathfrak{d}(x - z_\epsilon)\big). \tag{7.5}$$

We know obtain a positive lower bound independent of a for the flame eigenvalue c.

Theorem 7.5. *There exists a positive constant α independent of a such that*

$$\alpha \;\leq\; c. \tag{7.6}$$

Proof. We consider δ_1 small enough such that

$$\sqrt{\beta_0}\,\sqrt[4]{\delta_1} \leq \epsilon_1,$$

so that for $\delta \le \delta_1$ we have $z_{\epsilon_1} \le x_{\delta_1}$ from Lemma 7.2. We then consider the point $x_{\delta_1/2}$ which necessarily belongs to the interval (x_{δ_1}, a). Using the exponential estimates of Corollary 7.4 valid over $[z_{\epsilon_1}, a]$ we obtain that

$$c\delta_1/2 = \int_{x_{\delta_1/2}}^{a} \kappa \, dx \;\le\; (\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}}) c \exp\bigl(-\mathfrak{d}(x_{\delta_1/2} - z_{\epsilon_1})\bigr). \tag{7.7}$$

We also have

$$\sqrt{\beta_0}(\sqrt[4]{\delta_1} - \sqrt[4]{\delta_1/2}) \;\le\; \|\xi(z_{\epsilon_1}) - \xi^{\mathrm{e}}\| - \|\xi(x_{\delta_1/2}) - \xi^{\mathrm{e}}\| \;\le\; \|\xi(z_{\epsilon_1}) - \xi(x_{\delta_1/2})\|,$$

and letting $\alpha = \beta_0 \sqrt{\delta_1}\,(1 - 1/\sqrt[4]{2})^2$ we obtain from the entropic estimates

$$\alpha \;\le\; \Bigl(\int_{z_{\epsilon_1}}^{x_{\delta_1/2}} \|\xi'\| \, dx\Bigr)^2 \;\le\; (x_{\delta_1/2} - z_{\epsilon_1}) \int_{z_{\epsilon_1}}^{x_{\delta_1/2}} \|\xi'\|^2 \, dx \;\le\; \beta_2 c (x_{\delta_1/2} - z_{\epsilon_1}),$$

where β_2 is independent of a. This now yields that

$$\delta_1 \le 2(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}}) \exp\bigl(-\alpha_1/c\bigr),$$

where $\alpha_1 = \mathfrak{d}\alpha/\beta_2$ and the proof is complete. ∎

Note that in Proposition 7.3 and Theorem 7.5 we have only used the local version of the stability inequality concerning the chemical dissipation rate ζ.

7.2. Convergence towards equilibrium

Theorem 7.6. *There exists $\mathfrak{a}$, $\mathfrak{d}$ and $\mathfrak{C}$ independent of a such that*

$$\forall a \ge \mathfrak{a} \qquad \forall x \in [0, a], \qquad \|\xi(x) - \xi^{\mathrm{e}}\| \;\le\; \mathfrak{C} \exp(-\mathfrak{d} x), \tag{7.8}$$

Proof. In order to establish exponential convergence towards equilibrirum, we only have to establish that for a given $\epsilon > 0$, z_ϵ remains bounded independently of a. Let $0 < \epsilon < \epsilon_1$—where ϵ is determined later—and define $a_0\epsilon = \overline{c}(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}}) + 1$ where $\overline{c}$ is an upper bound for the eigenvalue c. Then, for $a \ge a_0$, there exists necessarily $x_0 \in [0, a_0]$ such that $\kappa(x_0) < \epsilon$. Since we have

$$\langle \phi, \phi \rangle \le b\kappa,$$

uniformly over $(-\infty, a]$ with b independent of a, we deduce that $\|\phi(x_0)\|^2 \le b\epsilon$. Since $Q(\xi - \xi^{\mathrm{e}}) = Q(\xi - \xi^{\mathrm{f}}) = -Q(\phi)$ where Q is the orthogonal projector onto $(0, M\mathcal{R})^\perp$, we can further use the global inequality of Proposition 3.15. This yields that $\sigma(\mathfrak{v}^{\mathrm{e}}) - \sigma \le \beta\epsilon$, so that

$$\|\mathfrak{v}^{\mathrm{e}} - \xi\|^2 \le \beta\epsilon.$$

In addition, we can also write that $\|\mathfrak{v}^{\mathrm{e}} - \xi^{\mathrm{e}}\| \le \beta\sqrt{\epsilon}$ since $Q(\xi - \xi^{\mathrm{e}}) = -Q(\phi)$. As a consequence, we obtain

$$\bigl\|\xi(x_0) - \xi^{\mathrm{e}}\bigr\|^2 \;\le\; \beta_3 \epsilon,$$

where β_3 is a constant. Assuming now $\epsilon < \epsilon_1/(1+\beta_3)$ we obtain that

$$\int_{x_0}^{a} \kappa\, du \ \leq\ \beta_1 \kappa(x_0) \leq \beta_1 \epsilon.$$

Further assuming $\beta_1\epsilon < \underline{c}(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}})$, then $x_{\beta_1\epsilon/\underline{c}}$ can be defined as in Lemma 7.1 and we have the estimate $x_{\beta_1\epsilon/\underline{c}} \leq a_0$. Letting

$$\bar{\epsilon} = \tfrac{1}{2} \inf\Bigl(\frac{\epsilon_1}{1+\beta_3}, \ \frac{\underline{c}\,(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}})}{\beta_1}, \ \frac{\underline{c}\,\epsilon_1^4}{\beta_0^2\beta_1}\Bigr),$$

we finally obtain from Lemma 7.2 that $z_{\bar{\epsilon}}$ is well defined with $\bar{\epsilon} < \epsilon_1$ and that

$$z_{\bar{\epsilon}} \leq a_0 = \bigl(\underline{c}\,(\sigma^{\mathrm{e}} - \sigma^{\mathrm{f}}) + 1\bigr)/\bar{\epsilon}.$$

Since $z_{\bar{\epsilon}}$ is bounded independently of a, we now obtain from Corrolary 7.4 that

$$\forall a \geq a_0, \qquad \forall x \in [0,a], \qquad \int_x^a \kappa\, du \leq \beta \exp(-\mathfrak{d} x),$$

and the proof is complete using again Lemma 7.2. ∎

Theorem 7.6 is the only place where the global inequality of Proposition 3.15 is used.

7.3. Passage to the limit $a \to \infty$

Theorem 7.7. *There exists a C^∞ solution to the anchored flame problem.*

Proof. We consider a sequence of solution (T^i, Y^i, c^i) of the anchored flame problem over the domains $[0,i]$ for $i \in \mathbb{N}\backslash\{0\}$. From the a priori estimates derived in Sections 5, 6 and 7, we can extract a subsequence converging towards (T, Y, c) on every compact in the C^2 topology. We then know that $\alpha < T < \beta$ and $\alpha < c < \beta$, where α and β are independent of i, and that $Y \geq 0$, $\langle Y, U \rangle = 1$. From the uniform L^2 estimates of derivatives, we easily deduce that T', Y', T'' and Y'' are in L^2 and from the exponential estimates, we also deduce that $\xi(\infty) = \xi^{\mathrm{e}}$. As a consequence, we conclude that (T, Y, c) is a solution of the anchored flames problem and from Lemma 5.1 we also obtain that $Y > 0$. Finally, the C^∞ regularity follows from the C^2 regularity and the governing equations. ∎

Note that the estimates obtained in Section 6 on a bounded domain $[0,a]$ could also be conducted directly over $[0,\infty)$.

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APPENDIX : Generalized Stefan-Maxwell -Boltzmann equations

The kinetic theory of gases yields explicit expressions for transport fluxes but not for transport coefficients. Transport linear systems have indeed to be solved in order to evaluate transport coefficients in gaseous mixtures. In this Appendix, we focus on the simplest linear systems associated with multicomponent diffusion coefficients and relate these systems to the so called Stefan-Maxwell-Boltzmann equations [Gio91] [EG94].

A.1 The matrices Δ and D

The transport linear systems associated with the multicomponent diffusion coefficients D are the n linear systems of order n indexed by l, $l \in S$,

$$\begin{cases} \Delta x^l = y^l, \\ \quad x^l \in Y^\perp, \end{cases} \tag{A.1}$$

where $\Delta \in \mathbb{R}^{n,n}$ and $x^l, y^l, Y \in \mathbb{R}^n$. The matrix Δ is given by

$$\begin{cases} \Delta_{kk} = \displaystyle\sum_{\substack{l \in S \\ l \neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}}, \qquad k \in S, \\ \\ \Delta_{kl} = -\dfrac{X_k X_l}{\mathcal{D}_{kl}}, \qquad k, l \in S, \quad k \neq l, \end{cases} \tag{A.2}$$

where $\mathcal{D}_{kl}$ is the binary diffusion coefficient for the species pair (k, l) when first order diffusion coefficients are considered [Gio91]. In this situation, the binary coefficients $\mathcal{D}_{kl}$, $k, l \in S$, only depends on pressure and temperature $\mathcal{D}_{kl} = \mathcal{D}_{kl}(T, p)$. More generally, for more accurate multicomponent diffusion coefficients, the quantities $\mathcal{D}_{kl}$, $k, l \in S$, are obtained as Schur complements from transport linear systems of size larger than n, and are then function of T, p, and Y, but have similar properties [EG94].

The right members y^l, $l \in S$, are given by

$$y_k^l = \delta_{kl} - \frac{Y_k}{\sum_{m \in S} Y_m}, \qquad k \in S, \tag{A.3}$$

where δ_{kl} is the Kronecker symbol. Finally, the diffusion coefficients D_{kl}, $k, l \in S$, are evaluated by

$$D_{kl} = x_k^l, \qquad k, l \in S. \tag{A.4}$$

The relations $(A.1)$ can easily be rewritten in terms of the species diffusion velocities $V_k = -\sum_{l \in S} D_{kl} \gamma_l'$ and yields

$$\gamma_k' = \sum_{\substack{l \in S \\ l \neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}} V_l \; - \; \Big(\sum_{\substack{l \in S \\ l \neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}}\Big) V_k, \qquad k \in S, \tag{A.5}$$

termed Stefan-Maxwell-Boltzmann equations in the literature. These equations have to be completed by the mass constraint

$$\sum_{k\in S} Y_k V_k = 0. \tag{A.6}$$

as the transport linear systems ($A.1$). However, although one may work with diffusion velocities and system ($A.5$), it is more elegant and more efficient to work directly with the transport coefficients [Gio91].

The matrix Δ is easily shown to have the following properties [Gio91] [EG94] [EG97].

Lemma A.1. *Assume that the molar masses m_k, $k \in S$, are positive constants, that the coefficients $\mathcal{D}_{kl}$ are positive and symmetric, and that the mass fractions Y are positive. Then Δ is symmetric positive semi-definite, $N(\Delta) = \mathbb{R}U$ where $U = (1,\ldots,1)^\star$, $R(\Delta) = U^\perp$, and $y^l \in R(\Delta)$, $l \in S$. Moreover, Δ is irreducible and is a singular M matrix.*

The matrix D is then easily related to a generalized inverse of Δ with prescribed range and nullspace [Gio90] [Gio91] [EG94] [EG97].

Proposition A.2. *Keep the assumptions of Lemma A.1. Then the n linear systems are well posed and the matrix D is the generalized inverse of Δ with prescribed range $Y^\perp$ and nullspace $\mathbb{R}Y$. More specifically, D is the the unique matrix such that $D\Delta D = D$, $\Delta D\Delta = \Delta$, $R(D) = Y^\perp$ and $N(D) = \mathbb{R}Y$. As a consequence, the matrix D is positive semi-definite, we have $\Delta D = I - Y\otimes U/\langle U,Y\rangle$, $D\Delta = I - U\otimes Y/\langle U,Y\rangle$, and for any positive a and b with $ab\langle U,Y\rangle^2 = 1$ we have $D = (\Delta + aY\otimes Y)^{-1} - bU\otimes U$.*

A.2 The matrices Γ and C

When some mass fraction are vanishing, the diffusion velocities are no longer defined and we have to consider the mass fluxes [Gio91]. As a consequence, we introduce the matrix Γ defined by

$$\begin{cases} \Gamma_{kk} = \dfrac{1}{\rho}\dfrac{\overline{m}}{m_k}\displaystyle\sum_{\substack{l\in S\\ l\neq k}} \dfrac{X_l}{\mathcal{D}_{kl}}, & k \in S, \\[2ex] \Gamma_{kl} = -\dfrac{1}{\rho}\dfrac{\overline{m}}{m_l}\dfrac{X_k}{\mathcal{D}_{kl}}, & k,l \in S, \quad k \neq l, \end{cases} \tag{A.7}$$

which satisfies $\Delta = \Gamma(\rho\mathcal{Y})$ [Gio91] . The transport linear systems associated with the flux diffusion coefficients C are the n linear systems of order n indexed by l, $l \in S$,

$$\begin{cases} \Gamma\tilde{x}^l = y^l, \\ \tilde{x}^l \in U^\perp, \end{cases} \tag{A.8}$$

and the flux diffusion coefficients C_{kl}, $k,l \in S$, are evaluated by

$$C_{kl} = \tilde{x}^l_k, \qquad k,l \in S. \tag{A.9}$$

One can also write the analog of equations $(A.5)$ for multicomponent fluxes $\gamma' = -\Gamma\mathcal{F}$ with the constraint $\mathcal{F} \in U^\perp$ [Gio91].

Lemma A.3. *Assume that the molar masses m_k, $k \in S$, are positive numbers, let $\mathcal{D}_{kl}$ be positive numbers defined for $k, l \in S$, $k \neq l$, and symmetric, i.e., $\mathcal{D}_{kl} = \mathcal{D}_{lk}$, for $k \neq l$, and assume that $Y \geq 0$ and $Y \neq 0$. Then the matrix Γ is such that $N(\Gamma) = \mathbb{R}Y$ and $R(\Gamma) = U^\perp$ and is a singular M-matrix.*

Proposition A.4. *Keep the assumptions of Lemma A.3. Then the n linear systems (A.8) are well posed and C is the group inverses of Γ, that is, C is the generalized inverse of Γ with prescribed range $U^\perp$ and prescribed nullspace $\mathbb{R}Y$. The matrix C is thus the unique matrix such that $C\Gamma C = C$, $\Gamma C \Gamma = \Gamma$, $R(C) = U^\perp$ and $N(C) = \mathbb{R}Y$. We also have $C\Gamma = \Gamma C = I - Y \otimes U / \langle U, Y \rangle$ and for any positive a and b with $ab\langle U, Y\rangle^2 = 1$ we have $C = (\Gamma + aY\otimes U)^{-1} - bY\otimes U$. Finally, when all mass fractions are positive, we have the identity*

$$C = \rho \mathcal{Y} D. \tag{A.10}$$

The next proposition gives the behavior of the matrices Γ and C when some of the mass fractions are vanishing [Gio91] [EG94].

Proposition A.5. *Keep the assumptions of Lemma A.3 and define $S^+ = \{\ k \in S,\ Y_k > 0\ \}$ and $S^0 = \{\ k \in S,\ Y_k = 0\ \}$. Let Υ be the permunation matrix associated with the reordering of S into (S^+, S^0). We then have the following block decompositions for C and Γ*

$$\Upsilon^\star C \Upsilon = \begin{pmatrix} C^{++} & C^{+0} \\ 0 & C^{00} \end{pmatrix}, \qquad \Upsilon^\star \Gamma \Upsilon = \begin{pmatrix} \Gamma^{++} & \Gamma^{+0} \\ 0 & \Gamma^{00} \end{pmatrix}, \tag{A.11}$$

where C^{00} and Γ^{00} are diagonal with positive entries and inverse of each other, and C^{++} and Γ^{++} are exactly the matrices that would be obtained by considering only the S^+ mixture of nonzero mass fractions. In particular, the matrices C^{++} and Γ^{++} satisfy the properties of Lemmas A.1 and A.3, and Propositions A.2 and A.4, for the submixture S^+.

A.3 Irreducibility and diagonal diffusion

In this section, we investigate the irreducibility of multicomponent diffusion matrices and the diagonal diffusion problem. Irreducibility is directly deduced from the assumptions of Section 4.

Proposition A.6. *The flux diffusion matrix C is irreducible if and only is $Y > 0$ so that the diffusion matrix D is always irreducible.*

Proof. From Proposition A.4 we already know that when some mass fractions are vanishing, the matrix C is reducible. As a consequence, we only have to establish that the converse is true. We assume that C is reducible so that there exists a permutation matrix Π such that

$$\Pi^\star C \Pi = \begin{pmatrix} C^{aa} & C^{ab} \\ 0 & C^{bb} \end{pmatrix},$$

where the superscripts ^{a} and ^{b} are used to denote the reordering associated with Π. Since $R(C) = U^\perp$, we deduce that $R(\Pi^\star C \Pi) = U^\perp$ so that $R(C^{aa}) \subset (U^a)^\perp$. This shows that C^{aa} is singular so that there exists $x^a \neq 0$ such that $C^{aa}x^a = 0$. Introducing the vector $x = (x^a, 0)^\star$, we obtain that $\Pi^\star C \Pi x = 0$ which yields $\Pi x \in N(C) = \mathbb{R}Y$. We have thus shown that $\Pi(x^a, 0)^\star = \alpha Y$ and α cannot be zero since $x^a \neq 0$ so that finally $Y = (1/\alpha)\Pi^\star(x^a, 0)^\star$ and some mass fractions are vanishing. ∎

We have shown in Proposition A.6 that the matrix C is irreducible when $Y > 0$ and this matrix cannot a fortiori be diagonal. However, we may ask for a weaker property since the physical vectors—the diffusion driving forces—always lie in the hyperplane $U^\perp$. Only the property of being represented by diagonal matrix over $U^\perp$ is needed. Moreover, a diagonal diffusion model is only interesting if the fluxes are expressed in terms of the mass fractions gradients which are the natural species variables. We have thus to investigate when the matrix $C\,(d_Y\gamma)$ is diagonal over $U^\perp$. However, since

$$d_Y\gamma = \frac{1}{\langle Y, U\rangle}\Big(I - \frac{X\otimes U}{\langle Y, U\rangle}\Big)\, A$$

we have $(d_Y\gamma)x = Ax/\langle Y, U\rangle$ for $x \in U^\perp$ since $A^\star U = U$. It is thus equivalent to investigate the case where CA is diagonal over $U^\perp$ and this problem has been solved in [Gio91].

Proposition A.7. *The matrix CA coincides with a diagonal matrix on the subspace $U^\perp$ if and only if the numbers $\mathcal{D}_{kl}$, $k, l \in S$, $k \neq l$, are equal. In this situation we have*

$$CA = \mathcal{D}\Big(I - \frac{Z\otimes U}{\langle U, Y\rangle}\Big), \qquad (A.12)$$

where $\mathcal{D}$ denotes the common value of the $\rho\mathcal{D}_{kl}/\langle U, Y\rangle$ for $k \neq l$ and $Z = A^{-1}Y$.

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$$\sigma(h, Y) = \sigma\big(\Xi(T, Y)\big) = s(T, Y). \tag{3.2}$$

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$$c\,\langle Y, u\rangle' + \langle \mathcal{F}, u\rangle' = 0. \tag{3.25}$$

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$$\Xi^{-1}\big(h^{\mathrm{f}}, \mathfrak{X}\big) \ \subset\ \{\ (T, Y);\ \alpha \le T,\ Y \ge 0,\ \langle Y, U\rangle = 1\ \},$$

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$$d_k = \frac{C_{kk}}{\langle Y, U\rangle}\frac{\overline{m}}{m_k}, \tag{4.11}$$

$$\pi_k = -\frac{C_{kk}}{m_k}\Big(\sum_{l\in S}\frac{Y_l}{m_l}\Big)^{-2}\sum_{\substack{l\in S\\ l\neq k}}\frac{Y_l'}{m_l} + \frac{C_{kk}}{m_k}\widetilde{\chi}_k\Big(\sum_{l\in S}\frac{Y_l}{m_l}\Big)^{-1}\frac{T'}{T} + \sum_{\substack{l\in S\\ l\neq k}}\rho D_{kl}\big(\gamma_l' + \gamma_l\widetilde{\chi}_l(T'/T)\big), \tag{4.12}$$

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$$\big\langle(\partial_\xi^2\sigma)\xi', \phi\big\rangle = \big\langle(\partial_\xi\sigma)', \phi\big\rangle = \Big(\frac{1}{T}\Big)'q - \sum_{k\in S}\Big(\frac{g_k}{T}\Big)'\mathcal{F}_k,$$

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$$c\sum_{k\in S}Y_k^{\mathrm{f}}(h_k - h_k^{\mathrm{f}}) - \lambda T' + cRT\sum_{k\in S}\frac{\widetilde{\chi}_k}{m_k}Y_k^{\mathrm{f}} = 0.$$

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... and h by $\int_0^T c_p du + \sum_{k\in S} h_k(0)Y_k$. That is ...

$$\Big(c_pT' + \sum_{k\in S} h_k(T)Y_k',\, Y'\Big)^\star = \mathcal{L}^\sharp\Big(c\Big(\int_0^T c_p dx + \sum_{k\in S} h_k(0)Y_k,\, Y\Big)^\star - c\xi^{\mathrm{f}} - \int_0^x w(u)\,du\Big),$$

$$\Big(\widetilde{c}_pt' + \sum_{k\in S} h_k y_k', y'\Big)^\star = \widetilde{\mathcal{L}}^\sharp\Big(c\Big(\int_0^t \widetilde{c}_p dx + \sum_{k\in S} h_k(0)y_l, y\Big)^\star - c\xi^{\mathrm{f}} - \tau\int_0^x \widetilde{w}(u)\,du\Big), \quad (6.5)$$

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$$\big|\sigma'\langle\partial_\xi\sigma,\phi\rangle\big| = \Big|c_p\frac{T'}{T} + \sum_{k\in S} s_kY_k'\Big|\;\Big|-\lambda\frac{T'}{T} + \sum_{k\in S}(s_k + R\frac{\widetilde{\chi}_k}{m_k})\mathcal{F}_k\Big|,$$

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$$c(\sigma-\sigma^{\mathrm{f}}) + \langle\partial_\xi\sigma,\phi\rangle = \int_{-\infty}^x \kappa\,du \ge \int_{-\infty}^0 \kappa\,du = c\Big(\sigma(0) - \sigma^{\mathrm{f}} - \big\langle\partial_\xi\sigma(0), \xi(0)-\xi^{\mathrm{f}}\big\rangle\Big).$$

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$$c^2\int_0^1\Big(\big\|\xi-\xi^{\mathrm{f}} - \frac{\tau}{c}\int_0^x w\,du\big\|^2 + \big|\frac{1}{c}\langle\partial_\xi\sigma,\phi\rangle\big|^2\Big)\,dx \;\le\; bc.$$

$$|T(a)-T(0)| \;\le\; \int_0^a |T'(x)|\,dx \;\le\; \sqrt{a}\left(\int_0^a |T'(x)|^2\,dx\right)^{1/2},$$

$$T^{\mathrm{e}} - T^{\mathrm{i}} \;\le\; b\sqrt{a}\left(\int_0^a \kappa\,dx\right)^{1/2} \;\le\; b\sqrt{c}\sqrt{a},$$

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$$\Big(\widetilde{c}_p^{\,\tau}\,t' + \sum_{k\in S} h_k^\tau\,y_k',\; y'\Big)^\star = (\widetilde{\mathcal{L}}^\tau)^\sharp\Big(c\Big(\int_0^t \widetilde{c}_p^{\,\tau} dx + \sum_{k\in S} h_k(0)y_k,\; y\Big)^\star - c\,\xi^{\mathrm{f},\tau}\Big), \qquad (6.17)$$

$$\widetilde{\mathcal{C}}^\tau = \tau\widetilde{\mathcal{C}} + (1-\tau)\overline{D}\Big(I\langle\widetilde{Y},U\rangle - \widetilde{Y}\otimes U\Big),$$

$$\xi^{\mathrm{f},\tau} = \Big(\sum_{k\in S} Y_k^{\mathrm{f}}\big(h_k(0) + \int_0^{T^{\mathrm{f}}} \widetilde{c}_{pk}^{\,\tau} dx\big),\ Y^{\mathrm{f}}\Big)^{\star},$$

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$$\xi^{\mathrm{e},\tau} = \Big(\sum_{k\in S} Y_k^{\mathrm{e}}\big(h_k(0) + \int_0^{T^{\mathrm{e}}} \widetilde{c}_{pk}^{\,\tau} dx\big),\ Y^{\mathrm{e}}\Big)^{\star},$$

On page 50 (Missing references)

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