GLOBAL EXISTENCE FOR FULLY NONLINEAR REACTION-DIFFUSION SYSTEMS DESCRIBING MULTICOMPONENT REACTIVE FLOWS

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Abstract. We consider combustion problems in the presence of complex chemistry and nonlinear diffusion laws leading to fully nonlinear multispecies reaction-diffusion equations. We establish results of existence of solution and maximum principle, i.e. positivity of the mass fractions, which rely on specific properties of the models. The nonlinear diffusion coefficients are obtained by resolution of the so-called Stefan-Maxwell equations.

1. Introduction

In this paper we investigate some mathematical issues arising in the context of the coupling of multi-species exothermic chemical reactions to fluid motion. The physical paradigm for this problem is combustion. Another related important problem is that of multi-species endothermic chemical reactions, with applications for instance to the chemistry of the high atmosphere; this problem will be studied elsewhere, and we concentrate here on exothermic chemical reactions and combustion.

Mathematical models for multi-species chemical reactions almost exclusively deal with the special case of chemical species whose binary diffusion coefficients are constants all equal to one another. For it is only in that case that the coefficients of the Laplacians in the reaction-diffusion equations are simply those diffusion constants; see for instance [MMT93] and the references therein.

In the present article we are concerned with the more general case, more physically relevant, for which the binary coefficients differ from pair to pair, the constraint of momentum conservation, i.e. the vanishing of the sum of diffusion fluxes, leading to inescapable nonlinear coefficients associated with the second spatial derivatives in the reaction-diffusion equations governing the evolution of the chemical species. The situation is further complicated by the fact that here the linear relationship between the diffusion velocities of the various species and the concentration gradients of those species is given by the resolution of a singular linear system expressing the so-called Stefan-Maxwell equations [Max67], [Ste71], [BSL07], [Wil88].

As a result, it is not all clear if the equations governing the evolution of the various chemical species, yield solutions that are physically meaningful as well as mathematically sound. Such questions as boundedness, positive invariance and existence deserve to be addressed. It is that which is the subject of this article. The connection with the motion induced by these more general exothermic reactions is examined as well.

From the mathematical viewpoint the system of equations that we consider in space dimension $n = 2$ or $3$ consists of the following:

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- the Navier-Stokes equations for incompressible fluid corresponding to pressure and velocity \( p, \mathbf{v} \), for the mixture,
- the heat equation for the temperature \( \theta \) with a heat source term corresponding to the Arrhenius law,
- the evolution (conservation) equations for the mass fractions \( Y_1, \ldots, Y_N \), of the \( N \) species.

The boundary value problems that we study correspond to reasonable boundary conditions for a flame propagating upward in a vertical tube but it is clear that other related boundary value problems can be studied by similar methods.

As indicated before, the diffusion terms in these equations are nonlinear; for each of these equations it is a combination of \( \nabla Y_1, \ldots, \nabla Y_N \), with coefficients rational functions of \( Y_1, \ldots, Y_N \). These functions are not given explicitly; they are instead given by the resolution of the Stefan-Maxwell equations. In Section 3 we derive enough information on these coefficients to be able to conduct our theoretical study. The first rigorous mathematical study of the Maxwell-Stefan linear system can be found, to the best of our knowledge, in [Gio90], [Gio91] which mainly address questions of numerical computations; see also [EG94], [EG97], [Gio99], [Lar91] for the numerical computation of the diffusion coefficients and [WT62], [WU70] for the kinetic theory background.

The article is organized as follows. In Section 2 we describe the equations and the initial and boundary value problems and state the main results for the chemistry equations and for the complete system corresponding to the coupling with hydrodynamics. In Section 3 we study in details the Stefan-Maxwell equations considered as a singular linear algebraic system for the diffusion velocities \( \mathbf{V}_1, \ldots, \mathbf{V}_N \) or the corresponding fluxes \( \mathbf{F}_i \). We show there how to determine the diffusion fluxes \( \mathbf{F}_i \) in terms of the mass fractions \( Y_i \) and their gradients. These fluxes become singular when all \( Y_i \) vanish, a case that is necessary to handle in our mathematical investigation. A crucial tool in our approach is to define modified diffusion coefficients that yield the proper fluxes for the actual solutions of the Stefan-Maxwell diffusion equations and that remain regular when all the mass fractions \( Y_i \) tend to zero. Also we obtain enough information on the fluxes for our purpose and in particular to infer energy estimates from the equation for the Gibbs energy (see below). We conclude this section with explicit calculations for the relevant and interesting case of three species. In Section 4 we prove the results previously stated for the reaction-diffusion equations alone, assuming that the velocity and temperature are given. For that purpose we approximate the equations by more regular ones; these are equations for all mass fractions \( Y_i \) treated as formally independent unknowns for which the positivity conditions are not imposed. Afterwards we deduce that \( Y_i \geq 0 \) by using the maximum principle and show that \( \sum_{j=1}^N Y_j = 1 \). In order to pass to the limit, we then proceed with the fundamental energy estimate that results from the principles of thermodynamics involving the functions \( \log Y_i \) (Gibbs energy) [LL75]. This step requires a detailed study in particular due to the singularities in the log \( Y_i \) - terms. Our estimate allows us to pass to the limit, solving the exact equations. In Section 5 we couple the chemistry equations with the fluid and heat equations; we prove the existence result for the complete (coupled) system using the same method of regularization.

The main results in this article were announced in the note [MMT95], and a draft was written which was not completed at that time. After the passing away of Oscar Manley in 2001, the two others authors regained interest in this work in relation with recent developments on the subject, (see e.g. [Bot11], [BGS12], [JS13] and the references
therein), and with possible applications to the chemistry of the atmosphere. Additional noteworthy applications are listed in [JS13].

Concerning the mathematical analysis of the diffusion partial differential equations, local in time results can be found in [GM98a], [Bot11] while particular cases are considered in [BGS12], [GM98b] and [Bot11]. The general case is considered in [JS13] where the existence of solutions is derived for all time. In fact in [JS13] the results do not pertain to the usual (classical) system that we consider but to a formally equivalent system obtained in particular by assuming that $Y_i > 0$ at all time. Furthermore in [JS13] the quantity that we call $Y_M$ below, $Y_M = \sum_{i=1}^{N} Y_i/M_i$ is required to be constant. This assumption is licit when considering the isobaric isothermal case as done in [JS13] but not when coupling with hydrodynamics and combustion as we do here. Finally, in the approach of [JS13], the symmetry between the mass fractions $Y_1, \ldots, Y_N$ is broken by taking advantage of the relation $\sum_{i=1}^{N} Y_i = 1$ and eliminating one of the mass fractions, and other changes of variables are performed. Doing so the authors lose several structural properties of the system including the maximum principle for the mass fractions. On the contrary, a key point in our approach is to keep all the mass fractions, thus keeping the symmetry between the unknowns $Y_1, \ldots, Y_N$.

This article is dedicated to the memory of Oscar Manley who suggested this work and who was actively involved in it, with kind memories and our great appreciation for his scientific vision and his tremendous scientific culture.

2. The Equations and the Main Results

2.1. Description of the problem.

We consider a multi-component premixed gas flame propagating in a bounded channel $\Omega \subset \mathbb{R}^n$, $n = 2$ or $3$. We assume that $\Omega = (0, \ell) \times (0, h)$ if $n = 2$ and $\Omega = (0, \ell) \times (0, L) \times (0, h)$ if $n = 3$. We denote by $x = (x_1, x_2)$ or $(x_1, x_2, x_3)$ a generic point in $\mathbb{R}^2$ or $\mathbb{R}^3$ while $\{e_1, e_2\}$ or $\{e_1, e_2, e_3\}$ denotes the canonical orthonormal basis where $e_n$ is parallel to the ascending vertical. Under suitable assumptions (see [Wil88] or [MMT93]), and in particular assuming that the fluid is incompressible and using the Boussinesq approximation, the equations for the reactive flow read

(2.1) \[ \frac{\partial v}{\partial t} + (v \cdot \nabla)v - Pr \Delta v + \nabla p = e_n \sigma \theta, \]

(2.2) \[ \text{div } v = 0, \]

(2.3) \[ \frac{\partial \theta}{\partial t} + (v \cdot \nabla)\theta - \Delta \theta = - \sum_{i=1}^{N} h_i \omega_i(\theta, Y_1, \ldots, Y_N), \]

(2.4) \[ \frac{\partial Y_i}{\partial t} + (v \cdot \nabla)Y_i + \nabla \cdot F_i = \omega_i(\theta, Y_1, \ldots, Y_N), \quad 1 \leq i \leq N. \]

The unknowns, which are here in non-dimensional form, are the velocity $v = (v_1, v_2)$ or $(v_1, v_2, v_3)$, the pressure $p$, the temperature $\theta$ and the mass fractions $Y_i$ of the $N$ species involved in the chemical reactions. Furthermore $h_i, \sigma$ and $Pr$ (the Prandtl number) are positive constants. The structure of the $\omega_i$ which are given functions of $\theta, Y_1, \ldots, Y_N$, is described below, in (2.15)-(2.19). Naturally the mass fractions $Y_i$ are expected to satisfy the conditions

$Y_i \geq 0$ for $1 \leq i \leq N$, \[ \sum_{i=1}^{N} Y_i = 1. \]
We now discuss the form of the fluxes $F_i$. Our purpose is to study this problem in the case of complex multi-component diffusion laws. The fluxes $F_i$ in (2.4) read

$$F_i = Y_i V_i,$$

where $V_i$ is the diffusion velocity of species $i$, so that

$$\sum_{i=1}^{N} Y_i V_i = 0.$$

Under general assumptions, the diffusion velocities are given (implicitly) in terms of the gradients of the mole fractions $X_i$ by the Stefan-Maxwell equations (see [Max67], [Ste71], [BSL07], [Wil88]):

$$\nabla X_i = \sum_{j=1, j \neq i}^{N} d_{ij} X_i X_j (V_j - V_i), \quad i = 1, \ldots, N,$$

where $d_{ij} = \kappa / D_{ij}$ and $D_{ij} = D_{ji} > 0$ is the binary diffusion coefficient for species $i$ and $j$ while $\kappa$ is the thermal diffusion coefficient, here taken to be a constant. The resolution of (2.7) is not straightforward since this linear system (with respect to the $V_i$) has a singular matrix. Also, these equations involve the $X_i$ while equations (2.4) concern the mass fractions $Y_i$. The algebraic relations between the $X_i$ and the $Y_i$ are given in (2.14) below and in section 3 where we conduct a detailed study of the resolution of the Stefan-Maxwell equations. It is found there that the fluxes $F_i$ can be defined for arbitrary smooth (say $C^1$) functions $Y_i$ from $\Omega$ into $[0, +\infty)$, and have the form

$$F_i = -\sum_{j=1}^{N} a_{ij}(Y_1, \ldots, Y_N) \nabla Y_j, \quad \text{for } i = 1, \ldots, N,$$

with

$$\sum_{i,j=1}^{N} a_{ij}(Y_1, \ldots, Y_N) \nabla Y_j = 0. \quad \text{(2.9)}$$

The coefficients $a_{ij}$ are rational functions of $Y_1, \ldots, Y_N$, continuous from $[0, +\infty)^N$ into $\mathbb{R}$ and such that, for $i, j = 1, \ldots, N$,

$$a_{ij}(Y_1, \ldots, Y_N) = Y_i b_{ij}(Y_1, \ldots, Y_N), \quad \text{for } i \neq j,$$

where $b_{ij} : [0, +\infty)^N \to \mathbb{R}$ is continuous,

$$a_{ii}(Y_1, \ldots, Y_N) = b^0_i(Y_1, \ldots, Y_N) + Y_i b^1_i(Y_1, \ldots, Y_N),$$

where $b^0_i$ and $b^1_i : [0, +\infty)^N \to \mathbb{R}$ are continuous and $b^0_i(Y_1, \ldots, Y_N) \geq 0$.

Also the following property is proved to hold: there exists a constant $c_1 > 0$ such that

if $Y_1, \ldots, Y_N \in H^1(\Omega)$ are such that $0 \leq Y_i(x) \leq 1$ and

$$\sum_{j=1}^{N} Y_j(x) = 1 \quad \text{for a.e. } x \in \Omega,$$

then

$$-\sum_{i=1}^{N} F_i \cdot \nabla \mu_i 1_{(Y_i > 0)} \geq c_1 \sum_{i=1}^{N} |\nabla Y_i|^2, \quad \text{for a.e. } x \in \Omega,$$

\text{Property (2.9) is valid even if } \sum_{j=1}^{N} Y_j \neq 1; \text{ see (3.52) in Section 3.}
where \( \mathbb{1}_{(Y_i > 0)} \) is the characteristic function of the set \( \{ x \in \Omega, Y_i(x) > 0 \} \) and \( \mu_i = \mu_i(x) \) is only defined where \( Y_i(x) > 0 \) (or equivalently \( X_i(x) > 0 \)) by:

\[
\mu_i = \frac{1}{M_i} \log X_i, \text{ if } Y_i > 0.
\]

Here \( X_i \) is the mole fraction of species \( i \) given by

\[
X_i = \frac{Y_i}{M_iY_M}, \quad Y_M = \sum_{j=1}^{N} \frac{Y_j}{M_j}, \quad M_j = \text{molecular mass of species } j,
\]

and \( \nabla \mu_i \) is defined almost everywhere when \( Y_i \) (or \( X_i \)) > 0 by \( \nabla \mu_i(x) = \nabla X_i(x)/M_iX_i(x) \).

We will study equations (2.1)-(2.4) using the above properties of the fluxes \( F_i \). We show in Section 3 how the properties (2.8)-(2.12) can be actually proved for the fluxes \( F_i \) given by (2.5)-(2.7), or more precisely for suitably modified fluxes.

We now state the assumptions on the chemical rates \( \omega_i; \) \( \omega_i \) is the difference between the rate of production of species \( i \), \( \alpha_i = \alpha_i(\theta, Y_1, \ldots, Y_N) \geq 0 \), and the rate of removal of species \( i \); the rate of removal of species \( i \) is proportional to an integral power of \( Y_i \) and we write it in the form \( Y_i \beta_i(\theta, Y_1, \ldots, Y_N) \), with \( \beta_i \geq 0 \). Hence:

\[
\omega_i = \omega_i(\theta, Y_1, \ldots, Y_N) = \alpha_i(\theta, Y_1, \ldots, Y_N) - Y_i \beta_i(\theta, Y_1, \ldots, Y_N).
\]

We assume that the functions \( \alpha_i \) and \( \beta_i \) are defined for \( \theta \geq 0 \) and \( 0 \leq Y_k \leq 1 \), are continuous on \( \mathbb{R}_+ \times [0,1]^N \) and that

\[
\alpha_i(\theta, Y_1, \ldots, Y_N) \geq 0, \quad \beta_i(\theta, Y_1, \ldots, Y_N) \geq 0 \quad \text{for } \theta \geq 0, \; 0 \leq Y_k \leq 1,
\]

\[
\sum_{i=1}^{N} \omega_i(\theta, Y_1, \ldots, Y_N) = 0, \quad \text{for } \theta \geq 0, \; 0 \leq Y_k \leq 1,
\]

\[
\alpha_i, \beta_i \text{ and hence } \omega_i \text{ are bounded on } [0, +\infty) \times [0,1]^N,
\]

\[
\sum_{i=1}^{N} h_i \omega_i(0, Y_1, \ldots, Y_N) \leq 0, \quad \text{for } 0 \leq Y_k \leq 1.
\]

Note that these abstract assumptions are satisfied by the rates given by the Arrhenius law. See [MMT93] for specific examples.

Equations (2.1)-(2.4) are supplemented with appropriate boundary and initial conditions. We have set \( \Omega = (0, \ell) \times (0, h) \) for \( n = 2 \) and \( \Omega = (0, \ell) \times (0, L) \times (0, h) \) for \( n = 3 \). We assume that the flame propagates in the vertical \( x_n \) direction, the premixed reacting species entering from below. The vertical sides of the channel are adiabatically insulated and impervious to fluid flow. We denote by \( \Gamma_0 \) and \( \Gamma_h \) the parts of the boundary \( \partial \Omega \) of \( \Omega \) corresponding to \( x_n = 0 \) and \( x_n = h \) and we denote by \( \Gamma_\ell \) the lateral boundary corresponding to \( 0 < x_n < h \). Consequently, the boundary conditions read

\[
v_i = 0 \text{ on } \partial \Omega \text{ for } 1 \leq i \leq n - 1, \quad v_n = 1 \text{ on } \Gamma_0 \cup \Gamma_h, \quad \frac{\partial v_n}{\partial \nu} = 0 \text{ on } \Gamma_\ell,
\]

\[
\theta = 0 \text{ on } \Gamma_0, \quad \frac{\partial \theta}{\partial \nu} = 0 \text{ on } \Gamma_h \cup \Gamma_\ell,
\]

and for \( 1 \leq i \leq N \) :

\[
\begin{cases}
Y_i = Y_i^n \text{ on } \Gamma_0, \\
\nu \cdot F_i = 0 \text{ on } \Gamma_h \cup \Gamma_\ell,
\end{cases}
\]
that is for (2.22)$_2$:

\[(2.23)\quad \left( \sum_{j=1}^{N} a_{ij}(Y_1,\ldots,Y_N) \nabla Y_j \right) \cdot \nu = 0 \text{ on } \Gamma_h \cup \Gamma_{\ell}.\]

Here \(\nu = (\nu_1,\ldots,\nu_n)\) is the unit outward normal on \(\partial\Omega\) and \(Y_i^u\), \(1 \leq i \leq N\), is the concentration of the species \(Y_i\) as it enters the channel (unburnt gas). The \(Y_i^u\) are assumed to be constant and satisfy

\[(2.24)\quad Y_i^u > 0 \quad \forall i, \quad \sum_{i=1}^{N} Y_i^u = 1.\]

Finally, we associate with (2.1)-(2.4) and (2.20)-(2.22), the initial conditions

\[(2.25)\quad \nu(x,0) = \nu_0(x), \quad \theta(x,0) = \theta_0(x),\]

\[(2.26)\quad Y_i(x,0) = Y_{i,0}(x),\]

where we assume that

\[(2.27)\quad \theta_0(x) \geq 0,\]

\[(2.28)\quad Y_{i,0}(x) \geq 0, \quad \sum_{i=1}^{N} Y_{i,0}(x) = 1.\]

2.2. Existence results.

To state our existence results it is convenient to extend the domain of definition of the reaction rates \(\omega_i, 1 \leq i \leq N\), to \(\mathbb{R}^{N+1}\) by setting

\[(2.29)\quad \omega_i(\theta,Y_1,\ldots,Y_N) = \omega_i(\theta^+,\psi(Y_1),\ldots,\psi(Y_N)), \quad \theta \in \mathbb{R}, \quad Y_k \in \mathbb{R},\]

where, for \(s \in \mathbb{R}, s^+ = \max(s,0)\) and:

\[\psi(s) = s \text{ if } 0 \leq s \leq 1, \psi(s) = 1 \text{ if } s \geq 1, \psi(s) = 0 \text{ if } s \leq 0.\]

We first consider the system (2.4), assuming that \(\nu\) and \(\theta\) are given such that, for some \(T > 0:\)

\[(2.30)\quad \begin{cases} \nu \in L^\infty(0,T;L^2(\Omega)^n) \cap L^2(0,T;H^1(\Omega)^n), \\
\text{\(\nu\) satisfies (2.2) and the Dirichlet boundary conditions in (2.20).} \end{cases}\]

\[(2.31)\quad \theta \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)).\]

The following existence result holds.

**Theorem 2.1.** Under the assumptions (2.8)-(2.12), (2.15)-(2.18), (2.24), let \(Y_0 = (Y_{i,0})_{1 \leq i \leq N}\) be given in \(L^2(\Omega)^N\) such that (2.28) holds for almost every \(x\) in \(\Omega\), and let \(\nu\) and \(\theta\) be given satisfying (2.30) and (2.31). Then, problem (2.4), (2.22), (2.26) possesses a solution \(Y = (Y_i)_{1 \leq i \leq N}\) such that

\[(2.32)\quad Y \in L^\infty(0,T;L^2(\Omega)^N) \cap L^2(0,T;H^1(\Omega)^N).\]

Furthermore, we have

\[(2.33)\quad 0 \leq Y_i(x,t) \leq 1 \quad \text{and} \quad \sum_{i=1}^{N} Y_i(x,t) = 1, \quad \text{for } t \in (0,T) \text{ and a.e. } x \in \Omega.\]
Remark 2.1. To be more precise the solution \( Y \) in the theorem 2.1 is a weak solution that satisfies the following variational formulation for \( 1 \leq i \leq N \):

\[
\left\langle \frac{\partial Y_i}{\partial t}, z_i \right\rangle + \int_\Omega [(v \cdot \nabla)Y_i]z_i \, dx + \sum_{j=1}^N \int_\Omega a_{ij}(Y_1, \ldots, Y_N) \nabla Y_j \cdot \nabla z_i \, dx = \int_\Omega \omega_i(\theta, Y_1, \ldots, Y_N) z_i \, dx, \quad \forall z_i \in H^1_{\Gamma_0}(\Omega),
\]

where

\[
H^1_{\Gamma_0}(\Omega) = \{ z \in H^1(\Omega), \ z = 0 \text{ at } x_n = 0 \},
\]

and \( \langle \cdot, \cdot \rangle \) denotes the duality product between \( H^1_{\Gamma_0}(\Omega) \) and its dual. We infer from (2.34) that \( Y \) satisfies

\[
\frac{\partial Y_i}{\partial t} \in L^2(0, T; H^1_{\Gamma_0}(\Omega)'), \quad \text{for } 1 \leq i \leq N,
\]

which together with (2.32) guarantees that \( Y \in C([0, T]; L^2(\Omega)^N) \).

We now consider the general system (2.1)-(2.4). The following existence result holds:

Theorem 2.2. In space dimension \( n = 2 \) or \( 3 \), under the assumptions (2.8)-(2.12), (2.15)-(2.19), (2.24), let

\[
v_0 \in L^2(\Omega)^n, \quad \theta_0 \in L^2(\Omega), \quad Y_0 = (Y_{i,0})_{1 \leq i \leq N} \in L^2(\Omega)^N
\]

be given such that (2.2), (2.27), (2.28) hold for almost every \( x \) in \( \Omega \) and

\[
v_0 \cdot \nu = v_n = 1 \text{ on } \Gamma_0 \cup \Gamma_h, \quad v_0 \cdot \nu = 0 \text{ on } \Gamma_e^n. \tag{2.26}
\]

Then, for any \( T > 0 \), the problem (2.1)-(2.4), (2.20)-(2.22), (2.25)-(2.26) possesses a solution \((v, \theta, Y)\) such that (2.30), (2.31), (2.32), (2.33) hold and

\[
\theta(x, t) \geq 0 \text{ for } t \in (0, T) \text{ and a.e. } x \in \Omega. \tag{2.35}
\]

Remark 2.2. Again the solution \((v, \theta, Y)\) given by Theorem 2.2 is to be understood as a weak solution satisfying a suitable variational formulation. The equations for \( Y \) are given by (2.34) while the ones for \( v \) and \( \theta \) can be written down in a standard way.

Remark 2.3. The regularity of the solutions and their uniqueness will be investigated in a separate work. Uniqueness can only be considered in space dimension 2 since, in space dimension 3, we encounter the difficulties of the incompressible Navier-Stokes equations in that space dimension. For the regularity, in space dimension 2, we immediately obtain from (2.1)-(2.3), and (2.31), (2.32), that:

\[
\begin{align*}
(2.36) \quad & v \in L^\infty(0, T; H^1(\Omega)^2) \cap L^2(0, T; H^2(\Omega)^2), \\
& \theta \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)),
\end{align*}
\]

if \( v_0 \in H^1(\Omega)^2 \) and \( \theta_0 \in H^1(\Omega) \) satisfy the Dirichlet boundary conditions in (2.20) and (2.21) (see e.g. [Tem77]).

Remark 2.4. From the mathematical point of view, Theorem 2.1 extends to all dimensions \( n \). Theorem 2.2 involving the coupling with the Navier-Stokes equations could extend to all dimensions \( n \) as well, with some adjustments for the Navier-Stokes equations as in [Lio69], see also [Tem77].

\[^2\text{Note that these conditions make sense because } \text{div} \ v_0 = 0 \text{ by (2.2), see e.g. [Tem77].} \]
3. The Stefan-Maxwell Equations and their Solution

In this Section 3, we study the fluxes given by (2.5)-(2.7). Also we introduce suitably modified fluxes which satisfy the properties (2.8)-(2.12). Finally we study explicitly the case of three species.

3.1. The chemical background.

We consider $N$ different chemical species and denote by $M_i$ the molecular mass of species $i$ and by $f_i = f_i(x, \xi, t)$ the velocity distribution function for molecules of species $i$. Hence

$$f_i(x, \xi, t)dxd\xi$$

denotes the probable number of molecules of type $i$ in the range $dx = dx_1 \ldots dx_n$ about the spatial position $x \in \mathbb{R}^n$ and with velocities in the range $d\xi = d\xi_1 \ldots d\xi_n$ about the velocity $\xi$ at time $t$.

The total number of molecules of kind $i$ per unit spatial volume at $(x,t)$ is denoted by $N_i = N_i(x,t)$:

$$N_i(x,t) = \int_{\mathbb{R}^n} f_i(x,\xi,t)d\xi, \ i = 1, \ldots, N.$$  

The molecular concentration of species $i$ is

$$C_i = N_i/A, \ i = 1, \ldots, N,$$

where $A$ is the Avogadro number.

The quantities that we will use and study are $\rho_i, Y_i, X_i$ defined as follows:

- $\rho_i$ is the density of species $i$ (mass per unit volume):

\begin{equation}
(3.1) \quad \rho_i = M_iN_i = AM_iC_i, \ i = 1, \ldots, N,
\end{equation}

and

$$\rho = \sum_{i=1}^{N} \rho_i,$$

is the total density. We assume incompressibility; hence the total density is constant in space and time

$$\rho = \rho_0.$$

- $Y_i$ is the mass fraction of species $i$:

\begin{equation}
(3.2) \quad Y_i = \frac{\rho_i}{\rho}, \ i = 1, \ldots, N,
\end{equation}

so that

\begin{equation}
(3.3) \quad 0 \leq Y_i \leq 1 \text{ for } 1 \leq i \leq N, \quad \sum_{i=1}^{N} Y_i = 1.
\end{equation}

- $X_i$ is the mole fraction of species $i$:

\begin{equation}
(3.4) \quad X_i = \frac{C_i}{C},
\end{equation}

where $C = \sum_{j=1}^{N} C_j$ is the total number of moles per unit volume. As for (3.3), we also have

\begin{equation}
(3.5) \quad 0 \leq X_i \leq 1 \text{ for } 1 \leq i \leq N, \quad \sum_{i=1}^{N} X_i = 1.
\end{equation}

Simple and useful relations between the $X_i$ and $Y_i$ are derived below. At this point, we proceed with the definition of kinematical quantities.
The average velocity of molecules of type $i$, at $x$ at time $t$, is given by

$$\bar{v}_i(x,t) = \frac{1}{N_i} \int_{\mathbb{R}^n} \xi f_i(x,\xi,t)d\xi.$$  

The mass-weighted average velocity of the mixture is

$$\bar{v} = \sum_{i=1}^{N} Y_i \bar{v}_i,$$

which is the ordinary flow velocity considered in fluid dynamics.

The relative velocity of species $i$ is given by

$$V_i(x,t) = \bar{v}_i(x,t) - v(x,t), \quad i = 1, \ldots, N,$$

and, due to (3.3) and (3.6), we have

$$\sum_{i=1}^{N} Y_i V_i = 0. \quad (3.7)$$

The Stefan-Maxwell equations express the gradients of the $X_i$ in terms of the $V_i$:

$$\nabla X_i = \sum_{j=1; j \neq i}^{N} d_{ij} X_i X_j (V_j - V_i), \quad i = 1, \ldots, N, \quad (3.8)$$

where $d_{ij} = \kappa / D_{ij} > 0$, and $D_{ij} = D_{ji}$, $i \neq j$, is the binary diffusion coefficient for species $i$ and $j$, while $\kappa$ is a constant representing thermal diffusion coefficients.

We are interested in the fluxes $F_i$ given by

$$F_i = Y_i V_i. \quad (3.9)$$

In particular, we aim to show that the $F_i$ can be determined in term of the $Y_j$ and $\nabla Y_j$ through equations (3.7) and (3.8) and the $X - Y$ relations, $X = (X_1, \ldots, X_N)$, $Y = (Y_1, \ldots, Y_N)$.

We conclude this section by describing the relations between the $X_i$ and $Y_i$. In view of (3.1), (3.2) and (3.4), we obtain for $i = 1, \ldots, N$

$$Y_i = \frac{M_i C_i}{\sum_{j=1}^{N} M_j C_j}, \quad X_i = \frac{C_i}{\sum_{j=1}^{N} C_j},$$

and setting

$$Y_M = \sum_{j=1}^{N} \frac{Y_j}{M_j}, \quad X_M = \sum_{j=1}^{N} M_j X_j, \quad (3.10)$$

we have

$$Y_M X_M = 1, \quad (3.11)$$

$$Y_i = \frac{M_i X_i}{X_M}, \quad X_i = \frac{Y_i}{M_i Y_M}, \quad (3.12)$$

Also, setting

$$\underline{M} = \min_{1 \leq i \leq N} M_i, \quad \overline{M} = \max_{1 \leq i \leq N} M_i, \quad \bar{M} = \overline{M}/\underline{M}, \quad (3.13)$$
(3.10) yields readily since $X_i \geq 0$, $Y_i \geq 0$, and $\sum_{i=1}^{N} Y_i = \sum_{i=1}^{N} X_i = 1$:

\begin{equation}
\frac{1}{M} \leq Y_M \leq \frac{1}{M}, \quad M \leq X_M \leq M.
\end{equation}

Next, we turn to some relations between the gradients of $X_i$ and $Y_i$. We assume for the moment that the $X_i$ and $Y_i$ are smooth functions (say $C^1$) of $(x, t)$ for $x \in \Omega$ and $t \in (0, T)$. In any event, the relations are pointwise relations, which are derived independently of the location $(x, t)$. From (3.12), we have

\begin{equation}
\nabla Y_i = \frac{M_i}{X_M} \nabla X_i - \frac{M_i X_i}{X_M^2} \nabla X_M,
\end{equation}

\begin{equation}
\nabla X_i = \frac{1}{M_i Y_M} \nabla Y_i - \frac{Y_i}{M_i (Y_M)^2} \nabla Y_M.
\end{equation}

Also, setting

$$
|\nabla X|^2 = \sum_{i=1}^{N} |\nabla X_i|^2, \quad |\nabla Y|^2 = \sum_{i=1}^{N} |\nabla Y_i|^2,
$$

we obtain

\begin{equation}
\frac{1}{2N(M)^2} |\nabla X| \leq |\nabla Y| \leq 2N(M)^2 |\nabla X|.
\end{equation}

Indeed, with (3.13)-(3.15),

$$
|\nabla Y_i| \leq \tilde{M} |\nabla X_i| + \tilde{M}^2 \sum_{j=1}^{N} |\nabla X_j| \leq 2\tilde{M}^2 \sum_{j=1}^{N} |\nabla X_j|,
$$

which gives readily the second inequality in (3.17). The proof of the first one is similar by making use of (3.16).

3.2. The fluxes $F_i$.

From the physical context the $i^{th}$ species is absent in a region where $Y_i = 0$, so that $V_i$ does not make sense and $F_i = 0$ in such a region. We will see how this is reflected in a purely algebraic study of the Stefan-Maxwell equations.

We start with some remarks concerning the linear equations (for the $V_i$) (3.7), (3.8). By making use of (3.12), let us rewrite them as

\begin{equation}
\sum_{i=1}^{N} Y_i V_i = 0
\end{equation}

\begin{equation}
B(Y)V = P,
\end{equation}

where

\begin{equation}
B_{ij}(Y) = \begin{cases} 
-d_{ij}' Y_j & \text{for } j \neq i, \\
-\sum_{k=1;k\neq i}^{N} d_{ik}' Y_k & \text{for } j = i,
\end{cases}
\end{equation}

with

$$
d_{ij}' = \frac{d_{ij}}{M_i M_j},
$$

and

$$
P = (P_1, \ldots, P_N), \quad P_i = -Y_M^2 \nabla X_i,$$
is given by (3.10) and (3.16) in terms of $Y$ and $\nabla Y$. Clearly, (3.18), (3.19) is a system of $N + 1$ vectorial equations with $N$ vectorial unknowns (vectors of $\mathbb{R}^n$). Also, the matrix $B(Y)$ is symmetric and semi-definite positive, since

$$(B(Y)V, V) = \sum_{i,j=1; i \neq j}^{N} d'_{ij}Y_iY_j(V_i - V_j) \cdot V_i,$$

(3.21)

$$= \sum_{i,j=1; i < j}^{N} d'_{ij}Y_iY_j|V_i - V_j|^2,$$

due to $d''_{ji} = d'_{ij}$.

It is worth mentioning also that

$$\sum_{i=1}^{N} B_{ij}(Y) = 0, \quad j = 1, \ldots, N; \quad \sum_{j=1}^{N} B_{ij}(Y) = 0, \quad i = 1, \ldots, N. \tag{3.22}$$

It follows from (3.21) that if all the $Y_i$ are strictly positive, the matrix $B(Y)$ has rank $N - 1$. In that case, since $\sum_{i=1}^{N} P_i = -Y^2_M \sum_{i=1}^{N} \nabla X_i = 0 \text{ (a.e.)}$ as $\sum_{i=1}^{N} X_i = 1$, the equations (3.19) are consistent, so that equations (3.18) and (3.19) determine uniquely the $V_i$. In summary, from a strictly algebraic point of view, if all $Y_i$ are strictly positive and

$$\sum_{i=1}^{N} P_i = 0, \tag{3.23}$$

equations (3.18), (3.19) uniquely determine $V_1, \ldots, V_N$.

If, say, $Y_1, \ldots, Y_k$ are $> 0$ and $Y_{k+1} = \ldots = Y_N = 0$, then, by inspection of the matrix $B(Y)$, we see, as before, that $V_1, \ldots, V_k$ are uniquely determined. The remaining equations for $V_{k+1}, \ldots, V_N$ have no solutions unless $P_i = 0, \quad i = k + 1, \ldots, N$, in which case the corresponding $V_i$ are arbitrary, and $F_i = Y_iV_i = 0$, for $i = k + 1, \ldots, N$.3 We come back below to the definitions of the $F_i$. If some of the $Y_i$ vanish, it is not possible to determine uniquely the $V_i$. However, we are only interested in defining the fluxes $F_i$ and we will show later on that this is indeed possible.

Since $Y_i \geq 0$ and $\sum_{i=1}^{N} Y_i = 1$ in the case of interest to us, we must continue to study the resolution of the linear system (3.18)-(3.19) in the case where $Y_i \geq 0 \quad \forall i$, while not all of the $Y_i$ vanish, and $P$ is a vector of $\mathbb{R}^{Nn}$, not necessarily equal to $-Y^2_M \nabla X$.

At this point, let us continue to study the case $Y_i > 0, \quad \forall i$. The above argument for existence and uniqueness clearly breaks the symmetry with respect to the unknowns $V_1, \ldots, V_N$, one of the equations in (3.19) being replaced by (3.18). To avoid this difficulty, we aim to give a different formulation of (3.18)-(3.19). For that purpose, let us introduce the quantity

$$(B(Y)V_i, V_i) + \gamma \left| \sum_{i=1}^{N} Y_i V_i \right|^2 = (\text{with (3.21)}) \tag{3.24}$$

$$= \sum_{i,j=1; i < j}^{N} d'_{ij}Y_iY_j|V_i - V_j|^2 + \gamma \left| \sum_{i=1}^{N} Y_i V_i \right|^2 .$$

3From the analytical point of view (by opposition to the algebraic point of view), in a region where $Y_i = X_i = 0, \quad P_i = -Y^2_M \nabla X_i = 0 \text{ a.e.}$. 

Combining these two equalities successively gives (3.18) and (3.19).

We aim now to address the general case where some but not all $Y_i$ vanish. As already mentioned, we cannot define $V_i$ in general but, as we will see, we can define the $F_i$. We assume again that the $P_i$ are arbitrary vectors of $\mathbb{R}^n$ ($P_i \neq -Y_M^2 \nabla X_i$) such that

$$
\sum_{i=1}^{N} P_i = 0,
$$

(3.30)

and $\gamma = \bar{d}'$, we infer from (3.24) that

$$
(B(Y)V, V) + \gamma \left| \sum_{i=1}^{N} Y_i V_i \right|^2 \geq \gamma \left\{ \sum_{i,j=1, i < j}^{N} Y_i Y_j (|V_i|^2 + |V_j|^2) + \sum_{i=1}^{N} Y_i^2 |V_i|^2 \right\}
$$

(3.25)

$$
\geq \gamma \sum_{i,j=1}^{N} Y_i Y_j |V_i|^2 = \gamma \left( \sum_{j=1}^{N} Y_j \right) \left( \sum_{i=1}^{N} Y_i |V_i|^2 \right).
$$

(3.27)

In particular, when all $Y_j$ are strictly positive, the problem

$$
C(Y)V = P,
$$

(3.28)

where $P = (P_1, \ldots, P_N)$, $P_i \in \mathbb{R}^n$, has a unique solution.

Note that this problem is equivalent to (3.18)-(3.19) when $\sum_{i=1}^{N} P_i = 0$ and all $Y_j$ are strictly positive (even if $\sum_{j=1}^{N} Y_j \neq 1$). Indeed, if $V$ is the solution of (3.18)-(3.19), then

$$
\sum_{j=1}^{N} C_{ij}(Y)V_j = \sum_{j=1}^{N} B_{ij}(Y)V_j + \gamma Y_i \sum_{j=1}^{N} Y_j V_j = P_i.
$$

Conversely, if $C(Y)V = P$, then, on the one hand, by adding the equations, we find that

$$
\sum_{i,j=1}^{N} C_{ij}(Y)V_j = \sum_{i=1}^{N} P_i = 0,
$$

(3.29)

while, on the other hand, since $\sum_{i=1}^{N} B_{ij}(Y) = 0$, we have

$$
\sum_{i,j=1}^{N} C_{ij}(Y)V_j = \sum_{i,j=1}^{N} B_{ij}(Y)V_j + \gamma \left( \sum_{i=1}^{N} Y_i \right) \sum_{j=1}^{N} Y_j V_j = \gamma \left( \sum_{i=1}^{N} Y_i \right) \sum_{j=1}^{N} Y_j V_j.
$$

Combining these two equalities successively gives (3.18) and (3.19).

Now (3.28) is an invertible system of $Nn$ equations for $Nn$ unknowns, which is symmetric with respect to the unknowns.
and, replacing $Y_iV_i$ by $F_i$, we rewrite (3.18)-(3.19) in the form

$$\sum_{i=1}^{N} F_i = 0, \quad (3.31)$$

$$\left( \sum_{k=1; k \neq i}^{N} d'_{yk} Y_k \right) F_i - Y_i \sum_{j=1; j \neq i}^{N} d'_{ij} F_j = P_i, \quad 1 \leq i \leq N. \quad (3.32)$$

We consider again $\gamma = d'_i$ as in (3.25) and rewrite the linear system (3.28), replacing $Y_iV_i$ by $F_i$. We obtain (compare to (3.32)):

$$\left( \sum_{j=1; j \neq i}^{N} d'_{ij} Y_j + \gamma Y_i \right) F_i - Y_i \sum_{j=1; j \neq i}^{N} (d'_{ij} - \gamma) F_j = P_i, \quad 1 \leq i \leq N. \quad (3.33)$$

As for (3.28), we show that, when (3.30) is satisfied, (3.31)-(3.32) is equivalent to (3.33). Indeed, it is clear that (3.31)-(3.32) imply (3.33). Conversely if the $F_i$ satisfy equations (3.33) then, by adding these equations for $i = 1, \ldots, N$, we obtain

$$\gamma \left( \sum_{i=1}^{N} Y_i \right) \left( \sum_{j=1}^{N} F_j \right) = \sum_{j=1}^{N} P_j. \quad (3.34)$$

Hence (3.31) follows from (3.30); then equations (3.33) reduce to equations (3.32).

We claim that (3.33) possesses a unique solution, even if (3.30) is not satisfied. Let us assume, say that $Y_1, \ldots, Y_k > 0$, while $Y_{k+1} = \ldots = Y_N = 0$; equations (3.33) give for $i = k + 1, \ldots, N,$

$$F_i = P_i/S_i, \quad \text{with} \quad S_i = S_i(Y) = \sum_{j=1}^{k} d'_{ij} Y_j, \quad i = k + 1, \ldots, N. \quad (3.35)$$

For $i = 1, \ldots, k$, the remaining system (3.33) reads

$$\left( \sum_{j=1; j \neq i}^{k} d'_{ij} Y_j + \gamma Y_i \right) F_i - Y_i \sum_{j=1; j \neq 1}^{k} (d'_{ij} - \gamma) F_j = P_i + Y_i \sum_{j=k+1}^{N} (d'_{ij} - \gamma) F_j, \quad (3.36)$$

where $\gamma = d'_i$ again. Writing $F_i = Y_iV_i$, the system (3.36) is similar to (3.28) and it can be shown in the same way that it defines the $F_i$, $i = 1, \ldots, k$, uniquely.

To summarize, we have shown that, for every $P = (P_1, \ldots, P_N) \in \mathbb{R}^{Nn}$, (3.33) possesses a unique solution $F = (F_1, \ldots, F_N)$, provided $Y_i \geq 0, \forall i$, and not all the $Y_i$ vanish. Furthermore, in view of (3.34), (3.31) holds if and only if (3.30) is assumed, and in this case (3.33) is equivalent to (3.31)-(3.32).

We summarize this study in the following theorem.
Theorem 3.1. Let $P_i, 1 \leq i \leq N$, be arbitrary vectors of $\mathbb{R}^n$ satisfying the physically relevant condition:
\[
\sum_{i=1}^{N} P_i = 0.
\]
We consider the Stefan-Maxwell equations rewritten in the form (3.18), (3.19) for the $V_i$, or in the form (3.31), (3.32) for the $F_i$, where $(Y_1, \ldots, Y_N) \in \mathbb{R}^N$ is given, with $Y_i \geq 0 \forall i$ and not all of the $Y_i$ vanish.

(i) If $Y_i > 0 \forall i$, these $N+1$ linear equations are consistent and define the $V_i$ and $F_i = Y_iV_i$ uniquely. Furthermore, the $V_i$ are the solutions of the linear system (3.28) which has a symmetric positive matrix.

(ii) If some of the $Y_i$ are zero but not all of them, say if $Y_1, \ldots, Y_k > 0, Y_{k+1} = \ldots = Y_N = 0, V_1, \ldots, V_k$ are uniquely defined and $V_{k+1}, \ldots, V_N$ are undetermined. In this case all the $F_i$ are uniquely determined and are given by (3.35) and the resolution of the linear system (3.36) of order $k$. Furthermore $F_{k+1} = \ldots = F_N = 0$ in the (relevant) case where $P_{k+1} = \ldots = P_N = 0$.

(iii) In all cases, the $F_i$ are uniquely determined and solutions of the linear system (3.33) which has an invertible matrix.

3.3. More about the fluxes.

We want now to derive some properties of the fluxes $F_i$ that are the solutions to the linear system (3.33). Obviously using Cramer’s rule, we can write
\[
F_i = \sum_{j=1}^{N} f_{ij}(Y_1, \ldots, Y_N)P_j,
\]
where the $f_{ij}$ are rational functions with respect to the $Y_j$, defined on $\mathbb{R}_+^N \setminus \{(0, \ldots, 0)\}$ where $\mathbb{R}_+^N = [0, +\infty)^N$. Also, comparing (3.35) and (3.37) we see that, for $i \neq j$, $f_{ij}$ vanishes at $Y_i = 0$, so that
\[
f_{ij}(Y_1, \ldots, Y_N) = Y_i \tilde{f}_{ij}(Y_1, \ldots, Y_N),
\]
where $\tilde{f}_{ij}$ is a rational function continuous on $\mathbb{R}_+^N \setminus \{(0, \ldots, 0)\}$.

Recall that if $Y_i > 0, \forall i$, then $F_i = Y_iV_i$ and the $V_i$ are solutions of (3.28). Since the matrix $C(Y)$ is definite positive, the inversion of (3.28) gives $V_i = \sum_{j=1}^{N} D_{ij}(Y)P_j$ where $D(Y) = C(Y)^{-1}$ is symmetric definite positive. In particular, since $D_{ii}(Y) \geq 0$, the decomposition (3.37) of $F_i = Y_iV_i$ is such that
\[
f_{ii}(Y) \geq 0 \text{ on } [0, +\infty)^N \text{ and, by continuity, on } \mathbb{R}_+^N \setminus \{(0, \ldots, 0)\}.
\]

Let us specialize this result to the case where the $Y_i$ are functions from $\Omega$ into $\mathbb{R}_+$, say of class $C^1$, such that $\sum_{i=1}^{N} Y_i(x) \neq 0$ at each point $x \in \Omega$ and $P_i = P_i(x) = -Y_M^2 \nabla X_i(x)$ where
\[
X_i = \frac{Y_i}{M_i Y_M}, \quad Y_M = \sum_{j=1}^{N} \frac{Y_j}{M_j} > 0.
\]
Then (3.37) becomes
\[
F_i = -\sum_{j=1}^{N} f_{ij}(Y_1, \ldots, Y_N)Y_M^2 \nabla X_j.
\]
Since $\sum_{i=1}^{N} X_i = 1^4$, (3.30) is satisfied so that (3.31) is satisfied too and reads

$$(3.42) \quad \sum_{i,j=1}^{N} f_{ij}(Y_1, \ldots, Y_N) \nabla X_j = 0.$$ 

Then we express the $\nabla X_j$ in terms of the $\nabla Y_\ell$:

$$\nabla X_j = \frac{\nabla Y_j}{M_j Y_M} - \frac{Y_j}{M_j Y_M^2} \sum_{\ell=1}^{N} \nabla Y_\ell \frac{M_\ell}{M_\ell},$$

and the fluxes $F_i$ become

$$(3.43) \quad F_i = -\sum_{j=1}^{N} \tilde{a}_{ij}(Y_1, \ldots, Y_N) \nabla Y_j,$$

$$(3.44) \quad \tilde{a}_{ij} = \frac{f_{ij} Y_M}{M_j} - \sum_{\ell=1}^{N} \frac{Y_\ell f_{i\ell}}{M_j M_\ell},$$

Therefore, we infer from the properties of the $f_{ij}$ that

$$(3.45) \quad \tilde{a}_{ij}(Y_1, \ldots, Y_N) = \begin{cases} Y_i a_{ij}^*(Y_1, \ldots, Y_N), & \text{if } i \neq j, \\ b_i^0(Y_1, \ldots, Y_N) + Y_i b_i^1(Y_1, \ldots, Y_N), & \text{if } i = j, \end{cases}$$

where

$$\begin{cases} a_{ij}^*, b_i^0 \text{ and } b_i^1 \text{ are rational functions of } Y_1, \ldots, Y_N, \\ \text{continuous in } \mathbb{R}^N_+ \setminus \{(0, \ldots, 0)\}, \text{ and } b_i^0 \geq 0. \end{cases}$$

Also since (3.43) is just a rewriting of (3.41), (3.42) implies

$$(3.47) \quad \sum_{i,j=1}^{N} \tilde{a}_{ij}(Y_1, \ldots, Y_N) \nabla Y_j = 0,$$

provided, as before, that the $Y_i$ are functions from $\Omega$ into $\mathbb{R}^N_+$ such that $\sum_{i=1}^{N} Y_i(x) \neq 0$ at each point $x \in \Omega$; in particular $\sum_{j=1}^{N} \nabla Y_j(x) = 0$ is not required for (3.47).

At this point we have shown that the Stefan-Maxwell equations allow us to define the fluxes $F_i$ (but not necessarily the $V_i$) provided that $Y_j \geq 0, \forall j$, and not all $Y_j$ vanish. For the mathematical study (see (2.8)-(2.11)) we will need the fluxes to be defined for $Y = (Y_1, \ldots, Y_N) = (0, \ldots, 0)$. Clearly if all $Y_i$ vanish, equations (3.18)-(3.19) are not valid since in (3.8) we can not express $X_i$ in terms of the $Y_j$ by (3.12) ($Y_M$ vanishes). This leads us to introduce modified expressions of the fluxes, that is modifications of the coefficients in (3.37) and (3.43). The new coefficients will be defined on all of $\mathbb{R}^N_+$ and the corresponding new fluxes will coincide with the previous ones, provided that

$$(3.48) \quad \sum_{j=1}^{N} Y_j = 1.$$ 

Since we will be able to show that the solution of (2.4) (supplemented with the boundary and initial conditions) satisfies (3.48), the fluxes in (2.4) will indeed be the ones given by the Stefan-Maxwell equations, so that our modification is licit.

Coming back to the expression (3.37) for the fluxes, the coefficients $f_{ij}(Y_1, \ldots, Y_N)$ are rational functions continuous on $\mathbb{R}^N_+ \setminus \{(0, \ldots, 0)\}$, but with a singularity at $(0, \ldots, 0)$.

---

$^4$By (3.40), $\sum_{i=1}^{N} X_i = 1$, is valid although $\sum_{i=1}^{N} Y_i$ may not be equal to one.
In order to preserve convenient properties of these coefficients, it is useful to rewrite the corresponding fractions with the same positive denominator

\[ f_{ij} = \frac{g_{ij}}{h}, \]

where the \( g_{ij} \) and \( h \) are polynomial functions of \( Y \), \( h \) does not vanish in \( \mathbb{R}^N_+ \setminus \{(0, \ldots, 0)\} \) and is positive \(^5\). Setting

\[ \tilde{f}_{ij} = \frac{h}{h + \left( \sum_{\ell=1}^{N} Y_{\ell} - 1 \right)^2} f_{ij}, \]

the new coefficients are rational functions of \( Y_{1}, \ldots, Y_{N} \), defined and continuous on all of \( \mathbb{R}^N_+ \) which coincide with \( f_{ij} \) if \( \sum_{j=1}^{N} Y_{j} = 1 \) and they satisfy properties analogous to (3.38) and (3.39). Also if we set

\[ F_i = \sum_{j=1}^{N} \tilde{f}_{ij}(Y) P_j, \]

we still have

\[ \sum_{i=1}^{N} F_i = 0 \text{ if } \sum_{i=1}^{N} P_i = 0. \] (3.49)

Next we replace \( \tilde{a}_{ij} \) in (3.44) by

\[ a_{ij} = \frac{h}{h + \left( \sum_{\ell=1}^{N} Y_{\ell} - 1 \right)^2} \tilde{a}_{ij} = \frac{\tilde{f}_{ij} Y_{M}}{M_j} - \sum_{\ell=1}^{N} \frac{Y_{\ell} \tilde{f}_{i\ell}}{M_{j} M_{\ell}}, \] (3.50)

The \( a_{ij} \) are rational functions of the \( Y_{\ell} \), continuous on all of \( \mathbb{R}^N_+ \), taking the same values as \( \tilde{a}_{ij} \) if \( \sum_{j=1}^{N} Y_{j} = 1 \). They satisfy properties analogous to (3.45) and (3.46). Furthermore, setting

\[ \tilde{F}_i = - \sum_{j=1}^{N} a_{ij}(Y_{1}, \ldots, Y_{N}) \nabla Y_{j}, \] (3.51)

we have \( \tilde{F}_i = F_i \) when \( \sum_{j=1}^{N} Y_{j} = 1 \), and

\[ \sum_{i=1}^{N} \tilde{F}_i = 0 \text{ since } \sum_{i=1}^{N} F_i = 0, \]
i.e.

\[ \sum_{i,j=1}^{N} a_{ij}(Y_{1}, \ldots, Y_{N}) \nabla Y_{j} = 0, \] (3.52)

even if \( \sum_{j=1}^{N} \nabla Y_{j}(x) \) does not vanish.

Relations (3.50) define the \( a_{ij} \) in (2.8). The smoothness assumptions as well as (2.9), (2.10) and (2.11) are satisfied. The fluxes (2.8) coincide with the ones given by the Stefan-Maxwell equations, provided that \( \sum_{i=1}^{N} Y_{i} = 1 \).

In summary we have proven the following:

\(^5\)That is \( a_{1}/b_{1}, \ldots, a_{N}/b_{N}, \) are written as fractions with denominator \( (b_{1} \ldots b_{N})^2 \).
Theorem 3.2. For \( i = 1, \ldots, N \), let \( Y_i \in C^1(\Omega) \) (resp. \( Y_i \in H^1(\Omega) \)) be given such that \( Y_i(x) \geq 0 \) and \( \sum_{i=1}^{N} Y_i(x) \neq 0 \) at each point \( x \in \Omega \) (resp. for a.e. \( x \in \Omega \)). Then the generalized fluxes \( \tilde{F}_i(x) \) are given by (3.51) where the \( a_{ij} \) are rational functions of the \( Y_i \) defined and continuous on all of \( \mathbb{R}^N_+ \).

Furthermore if \( \sum_{i=1}^{N} Y_i(x) = 1 \) for \( x \in \Omega \) (resp. for a.e. \( x \in \Omega \)), they coincide with the solutions of the linear system (3.31), (3.32) with \( P_i = -Y_M^2 \nabla X_i \) (and the Stefan-Maxwell equations).

Finally the \( a_{ij} \) satisfy the properties (2.9), (2.10) and (2.11).

The generalized fluxes \( \tilde{F}_i \) are the ones we consider in equation (2.4) and we will now denote them by \( F_i \) for the sake of simplicity. However note that they coincide with the solutions of the Stefan-Maxwell equations given by Theorem 3.1 only if \( \sum_{i=1}^{N} Y_i = 1 \).

There remains to derive the property (2.12).

3.4. The property (2.12).

We are now given \( N \) functions \( Y_1, \ldots, Y_N \) belonging to \( H^1(\Omega) \) such that \( 0 \leq Y_i(x) \leq 1 \) and \( \sum_{j=1}^{N} Y_j(x) = 1 \) for a.e. \( x \in \Omega \).

Let us first assume that \( x \in \Omega \) is such that \( Y_i(x) > 0 \) \( \forall i \) and \( \sum_{i=1}^{N} Y_i(x) = 1 \). Then, in view of Theorem 3.1 (i), the fluxes \( F_i \) read

\[
F_i = Y_i V_i,
\]

where \( V_i \) is the solution of (3.28) with \( P_i = -Y_M^2 \nabla X_i \), that is

\[
C(Y)V = -Y_M^2 \nabla X.
\]

Recalling the definition (2.13) for \( \mu_i \), we have

\[
-\sum_{i=1}^{N} F_i \cdot \nabla \mu_i = -\sum_{i=1}^{N} \frac{Y_i}{M_i X_i} V_i \cdot \nabla X_i,
\]

\[
= -Y_M \sum_{i=1}^{N} V_i \cdot \nabla X_i, \text{ with (3.12),}
\]

\[
= \frac{1}{Y_M} \sum_{i,j=1}^{N} C_{ij}(Y)V_j \cdot V_i, \text{ thanks to (3.53).}
\]

Since \( \sum_{j=1}^{N} Y_j(x) = 1 \), the coercivity property (3.27) for the matrix \( C(Y) \) reads

\[
\sum_{i,j=1}^{N} C_{ij}(Y)V_j \geq \gamma \left( \sum_{i=1}^{N} Y_i |V_i|^2 \right), \text{ with } \gamma = d',
\]

and the bounds (3.14) for \( Y_M \) hold true. Therefore we infer from (3.54) that

\[
\sum_{i=1}^{N} F_i \cdot \nabla \mu_i \geq \gamma M \sum_{i=1}^{N} Y_i |V_i|^2.
\]

Next, recall that \( V_i \) is also the solution of (3.19) with \( P_i = -Y_M^2 \nabla X_i \) so:

\[
-Y_M^2 \nabla X_i = \sum_{j=1}^{N} B_{ij}(Y)V_j,
\]
In view of the definition (3.20) of $B_{ij}$ and using again (3.14), we find

$$|\nabla X_i| \leq \frac{N}{M} \sum_{j=1}^{N} |B_{ij}(Y)||V_j|,$$

$$\leq \frac{d}{M} \sum_{k=1; k \neq i}^{N} Y_k |V_k| + \sum_{j=1; j \neq i}^{N} Y_i |V_j|,$$

(3.56)

$$\leq \frac{d}{M} Y_i^{1/2} \left( \sum_{k=1}^{N} |V_k|^2 \right)^{1/2} \left\{ \left( \sum_{k=1; k \neq i}^{N} Y_k \right) + \sum_{j=1; j \neq i}^{N} Y_j \right\}^{1/2},$$

$$\leq \frac{d}{M} Y_i^{1/2} (1 - Y_i)^{1/2} \left( \sum_{k=1}^{N} |V_k|^2 \right)^{1/2}.$$

Thanks to the relations (3.17) between $\nabla X$ and $\nabla Y$, we infer from (3.56) that

$$|\nabla Y|^2 = \sum_{i=1}^{N} |\nabla Y_i|^2 \leq c^2 \left( \sum_{i=1}^{N} Y_i |V_i|^2 \right),$$

(3.57)

where $c$ is an appropriate constant depending on $N, d, \tilde{M}, M$.

We conclude by combining (3.55) and (3.57). This provides

$$- \sum_{i=1}^{N} F_i \cdot \nabla \mu_i \geq c_1 |\nabla Y|^2.$$

Now, assume that $Y_{k+1} = \ldots = Y_N = 0$ and $Y_1, \ldots, Y_k > 0$ at some $x \in \Omega$ and for some $k \geq 1$. Then, for a.e. such $x \in \Omega$, since $Y_i \in H^1(\Omega)$, we have

$$\nabla Y_i(x) = 0, \quad \nabla X_i(x) = 0, \quad i = k + 1, \ldots, N$$

so that $P_{k+1} = \ldots = P_N = 0$. Therefore, in view of Theorem 3.1 (ii), $F_{k+1} = \ldots = F_N = 0$ while $F_1, \ldots, F_k$ are the solutions of

$$\left( \sum_{j=1; j \neq i}^{k} d'_{ij} Y_j + \gamma Y_i \right) F_i - Y_i \sum_{j=1; j \neq i}^{k} \left( d'_{ij} - \gamma \right) F_j = -Y_M^2 \nabla X_i, \quad i = 1, \ldots, k.$$

As already noticed, this system is similar to the previous one when all $Y_i$ are positive. Therefore, with computations similar to the ones above, we find

$$- \sum_{i=1}^{N} F_i \cdot \nabla \mu_i 1_{\{Y_i>0\}} = - \sum_{i=1}^{k} F_i \cdot \nabla \mu_i \geq c_1 \left( \sum_{j=1}^{k} |\nabla Y_j|^2 \right) = c_1 \left( \sum_{j=1}^{N} |\nabla Y_j|^2 \right).$$

The above inequalities valid for various values of $k$ provide (2.12).

Remark 3.1. Note that our method of solutions of the Stefan-Maxwell equations reducing first the problem to the inversion of a symmetric positive definite matrix (the matrix $C(Y)$ in (3.26)-(3.28)) is closely related to the one in [Gio90], [Gio91]. However our presentation above, contains some additional developments that are new to the best of our knowledge, in particular the generalized definition of the fluxes when all the $Y_i$ vanish, and the properties of these generalized fluxes, including the property (2.12).
3.5. The three species case.
We conclude this Section 3 by studying explicitly the three species case \((N = 3)\) which is of interest, as it includes for instance the evolution of ozone when the three species are atomic oxygen, molecular oxygen and ozone \((O, O_2, O_3\) respectively, see Appendix B in [MMT93]).

The matrix \(B(Y)\) in (3.20) is written
\[
(3.58) \quad B = \begin{pmatrix}
  b + c & -c & -b \\
  -c & a + c & -a \\
  -b & -a & a + b
\end{pmatrix},
\]
where
\[
(3.59) \quad a = d'_{23}Y_2Y_3, \quad b = d'_{13}Y_1Y_3, \quad c = d'_{12}Y_1Y_2.
\]

The resolution of (3.18)-(3.19) (or more precisely of (3.31)-(3.32)) is much simplified by observing that
\[
DB = \rho I - \begin{pmatrix}
  bc & ac & ab \\
  bc & ac & ab \\
  bc & ac & ab
\end{pmatrix},
\]
where \(D\) is the diagonal matrix \((a, b, c)\) and \(\rho = ab + bc + ca\), hence in view of (3.59):
\[
(3.60) \quad \rho = Y_1Y_2Y_3\tilde{\rho}, \quad \text{with} \quad \tilde{\rho} = d'_{13}d'_{23}Y_3 + d'_{12}d'_{13}Y_1 + d'_{12}d'_{23}Y_2.
\]
Here, when the \(Y_i\) are positive and at least one of them does not vanish, we have \(\tilde{\rho} > 0\).

Now, multiplying both sides of equation (3.19) by \(D\), we find
\[
(3.61) \quad \rho V - (\sigma, \sigma, \sigma)^T = (aP_1, bP_2, cP_3)^T,
\]
where \(\sigma = bcV_1 + acV_2 + abV_3\). Taking the scalar product of (3.61) with \(Y\) and using \(\sum_{i=1}^{3} Y_iV_i = 0\), we find
\[
\sigma = -\left(\sum_{i=1}^{3} Y_i\right)^{-1} (aY_1P_1 + bY_2P_2 + cY_3P_3),
\]
so that
\[
(3.62) \quad V = \frac{1}{\rho} \left(\frac{\sigma + aP_1}{\sigma + bP_2}\right).
\]
We recover that \(V\) is only defined when all \(Y_i\) are strictly positive. However, recalling that \(F_i = Y_iV_i\), we have:
\[
(3.63) \quad \begin{pmatrix}
  F_1 \\
  F_2 \\
  F_3
\end{pmatrix} = -\frac{1}{\rho} \sum_{i=1}^{3} Y_i \begin{pmatrix}
  d'_{23}Y_1P_1 + d'_{13}Y_1P_2 + d'_{12}Y_1P_3 \\
  d'_{23}Y_2P_1 + d'_{13}Y_2P_2 + d'_{12}Y_2P_3 \\
  d'_{23}Y_3P_1 + d'_{13}Y_3P_2 + d'_{12}Y_3P_3
\end{pmatrix},
\]
which is defined when \(Y_i \geq 0\) and not all of the \(Y_i\) vanish. This gives the explicit form of the coefficients \(f_{ij}\) in (3.37). We recover that they are rational functions defined and continuous on \(\mathbb{R}_+^N \setminus \{(0, \ldots, 0)\}\) and that they satisfy the properties (3.38) and (3.39).

Setting \(P_i = -Y_M^2 \nabla X_i\), and expressing the \(\nabla X_i\) in terms of the \(\nabla Y_j\) provide the coefficients in (3.43); the properties (3.45) and (3.46) follow as well.
4. The Chemistry System

The aim of this section is to study the problem (2.4) and to prove Theorem 2.1. For that purpose, we first introduce a modified problem depending on a parameter \( \varepsilon > 0 \) for which we obtain an existence result. Then we derive the existence of a solution of (2.4) by taking the limit \( \varepsilon \to 0 \).

4.1. The modified equations.

We first modify and extend the coefficients \( a_{ij} \) to be defined on \( \mathbb{R}^N \) by setting

\[
\hat{a}_{ij}(Y_1, \ldots, Y_N) = \xi \left( \sum_{\ell=1}^{N} |Y_\ell| \right) a_{ij}(Y_1^+, \ldots, Y_N^+), \quad 1 \leq i, j \leq N, \quad Y_k \in \mathbb{R},
\]

where \( \xi : \mathbb{R}_+ \to \mathbb{R}_+ \) is a continuous function such that

\[
\xi(s) = s \text{ if } 0 \leq s \leq 1, \quad \xi(s) \in [0, 1] \text{ if } 1 \leq s \leq 2, \quad \xi(s) = 0 \text{ if } s \geq 2.
\]

Clearly, the \( \hat{a}_{ij} \) are continuous bounded functions. The same is true for the \( \omega_i \) given by (2.29) and we set

\[
K_1 = \max_{i,j} \sup_{\mathbb{R}^N} |\hat{a}_{ij}|, \quad K_2 = \max_{i} \sup_{\mathbb{R}^{N+1}} |\omega_i|.
\]

For \( q > 2 \) fixed and for \( \varepsilon > 0 \) fixed (which we will let converge to zero later on), we consider the following modified form of (2.4):

\[
\frac{\partial Y_i}{\partial t} + (v \cdot \nabla) Y_i + \nabla \cdot \hat{F}_i - \varepsilon \nabla \cdot (|\nabla Y|^{q-2} \nabla Y_i) = \omega_i(\theta, Y_1, \ldots, Y_N), \quad 1 \leq i \leq N.
\]

Here, \( Y_i = Y_{i,\varepsilon} \) depends of course on \( \varepsilon \), but we omit to denote this dependence as long as \( \varepsilon \) is kept fixed. Also, \( |\nabla Y|^2 = \sum_{j=1}^{N} |\nabla Y_j|^2 \) and

\[
\hat{F}_i = -\sum_{j=1}^{N} \hat{a}_{ij}(Y_1, \ldots, Y_N) \nabla Y_j,
\]

where \( \hat{a}_{ij} \) is given by (4.1). We supplement (4.3) with the same boundary and initial conditions as before, namely (2.22) and (2.26) except that (2.22)_2 is replaced by

\[
\nu \cdot (\hat{F}_i - \varepsilon |\nabla Y|^{q-2} \nabla Y_i) = 0 \text{ on } \Gamma_h \cup \Gamma_\ell.
\]

To obtain the weak formulation of this problem we observe that \( Y_i - Y_i^\varepsilon \) vanishes at \( x_n = 0 \). Hence, upon multiplying (4.3) by a smooth test function \( z_i \) vanishing at \( x_n = 0 \), we obtain thanks to (4.5):

\[
\int_{\Omega} \frac{\partial Y_i}{\partial t} z_i dx + \int_{\Omega} [(v \cdot \nabla) Y_i] z_i dx + \sum_{j=1}^{N} \int_{\Omega} \hat{a}_{ij}(Y_1, \ldots, Y_N) \nabla Y_j \cdot \nabla z_i dx
\]

\[
+ \varepsilon \int_{\Omega} |\nabla Y|^{q-2} \nabla Y_i \cdot \nabla z_i dx = \int_{\Omega} \omega_i(\theta, Y_1, \ldots, Y_N) z_i dx, \quad 1 \leq i \leq N.
\]

Let us introduce the Sobolev space \( W^{1,q}(\Omega) \) and its subspace

\[
W^{1,q}_{\Gamma_0}(\Omega) = \{ z \in W^{1,q}(\Omega), \quad z = 0 \text{ at } x_n = 0 \}.
\]

We denote by \( (W^{1,q}_{\Gamma_0}(\Omega))' \) its dual, and \( < \cdot, \cdot > \) denotes the duality product between \( W^{1,q}_{\Gamma_0}(\Omega) \) and its dual. Subsequently we replace in (4.6)

\[
\int_{\Omega} \frac{\partial Y_i}{\partial t} z_i dx \quad \text{by} \quad < \frac{\partial Y_i}{\partial t}, z_i >.
\]
We now aim to prove the following existence result.

**Proposition 4.1.** Under the assumptions of Theorem 2.1, for \( q > 2 \) and \( \varepsilon > 0 \) given, problem (4.3), (4.5), (2.22) possesses a solution \( Y = (Y_1, \ldots, Y_N) \) such that

\[
Y_i \in L^\infty(0, T; L^2(\Omega)) \cap L^q(0, T; W^{1,q}(\Omega)),
\]

\[
\frac{\partial Y_i}{\partial t} \in L^q(0, T; (W_1^{1,q}(\Omega))^\prime), \quad \text{with} \quad \frac{1}{q} + \frac{1}{q} = 1.
\]

**Remark 4.1.** We do not require any positivity property for the solutions of (4.3). We will come back to this point later on.

**Proof.** Existence is based on the methods of compactness and monotonicity (see e.g. J.L. Lions [Lio69]) and on the following a priori estimate (only valid for \( \varepsilon > 0 \) fixed).

Replacing \( z_i \) by \( Y_i - Y_i^u \) in (4.6), we obtain

\[
\frac{1}{2} \frac{d}{dt} \int_\Omega (Y_i - Y_i^u)^2 dx + \int_\Omega [(\mathbf{v} \cdot \nabla) Y_i](Y_i - Y_i^u) dx
\]

\[
+ \sum_{j=1}^N \int_\Omega \hat{a}_{ij}(Y) \nabla Y_j \cdot \nabla Y_i dx + \varepsilon \int_\Omega |\nabla Y|^q |\nabla Y_i|^2 dx
\]

\[
= \int_\Omega \omega_\varepsilon(\theta, Y)(Y_i - Y_i^u) dx.
\]

The different terms in (4.9) can be estimated by making use of (2.30) and (4.2). We find

\[
\int_\Omega [(\mathbf{v} \cdot \nabla) Y_i](Y_i - Y_i^u) dx = \frac{1}{2} \int_\Omega (\mathbf{v} \cdot \nabla)(Y_i - Y_i^u)^2 d\Gamma - \frac{1}{2} \int_\Omega (Y_i - Y_i^u)^2 (\text{div } \mathbf{v}) dx
\]

\[
= \frac{1}{2} \int_{\Gamma_h} (Y_i - Y_i^u)^2 d\Gamma \geq 0.
\]

Also,

\[
\left| \sum_{j=1}^N \int_\Omega \hat{a}_{ij}(Y) \nabla Y_j \cdot \nabla Y_i dx \right| \leq K_1 \sum_{j=1}^N \int_\Omega |\nabla Y_j| |\nabla Y_i| dx,
\]

\[
\left| \int_\Omega \omega_\varepsilon(\theta, Y)(Y_i - Y_i^u) dx \right| \leq K_2 \int_\Omega |Y_i - Y_i^u| dx.
\]

Combining the above inequalities with (4.9) and adding for \( i = 1, \ldots, N \), we conclude that

\[
\frac{1}{2} \frac{d}{dt} \sum_{i=1}^N \int_\Omega (Y_i - Y_i^u)^2 dx + \varepsilon \int_\Omega |\nabla Y|^q dx \leq N K_1 \int_\Omega |\nabla Y|^2 dx
\]

\[
+ K_2 \left\{ \sum_{i=1}^N \int_\Omega |Y_i - Y_i^u| dx \right\}.
\]

This inequality readily yields, for fixed \( \varepsilon \), a priori bounds of \( Y_i - Y_i^u \) in \( L^\infty(0, T; L^2(\Omega)) \) and \( L^q(0, T; W_1^{1,q}(\Omega)) \).

Next, combining these bounds and the weak formulation (4.6) provide a priori bounds of \( \frac{\partial Y_i}{\partial t} \) in \( L^q(0, T; (W_1^{1,q}(\Omega))^\prime) \).

These estimates allow us to show the existence of a solution of (4.3), (4.5), (2.22) thanks to standard arguments: introduction of a Galerkin approximation and passage to the limit by monotonicity and compactness (see e.g. [Lio69], p. 207). \( \square \)
As already noticed, we did not require any positivity property for the \( Y_j \), when formulating the problem (4.3). We conclude this section by showing that in fact such properties hold for the solutions that we have obtained.

**Proposition 4.2.** Under the assumptions of Theorem 2.1, the solutions \( Y_i \) of (4.3), (4.5), (2.22), (2.26) satisfy

\[
\begin{align*}
0 & \leq Y_i(x,t) \leq 1, \text{ for } t \in [0,T] \text{ and a.e. } x \in \Omega, \\
\sum_{j=1}^N Y_j(x,t) & = 1, \text{ for } t \in [0,T] \text{ and a.e. } x \in \Omega.
\end{align*}
\]

**Proof.** To derive the positivity, we set \( z_i = -Y_i^- = \min(0, Y_i) \in W^{1,q}_T(\Omega) \) in (4.6) and we find after some integrations by parts and upon using (2.30):

\[
\frac{1}{2} \frac{d}{dt} \int_\Omega (Y_i^-)^2 dx + \frac{1}{2} \int_{\Gamma_h} (Y_i^-)^2 d\Gamma - \sum_{j=1}^N \int_\Omega \hat{a}_{ij}(Y) \nabla Y_j \cdot \nabla Y_i^- dx \\
+ \varepsilon \int_\Omega |\nabla Y|^q - 2 |\nabla Y_i^-|^2 dx = - \int_\Omega \omega_i(\theta, Y) Y_i^- dx.
\]

Now at each point \((x,t)\) such that \( Y_i(x,t) \leq 0\), the definition (4.1) of \( \hat{a}_{ij} \) together with the assumptions (2.10), (2.11) guarantee that

\[
- \sum_{j=1}^N \hat{a}_{ij}(Y_1, \ldots, Y_N) \nabla Y_j \cdot \nabla Y_i^- = \xi \left( \sum_{\ell=1}^N |Y_{\ell}| \right) b_i^0(Y_1^+, \ldots, Y_N^+) |\nabla Y_i^-|^2 \geq 0.
\]

while, the definition (2.29) of the extended \( \omega_i \) together with the assumptions (2.15), (2.16) provide that:

\[
\omega_i(\theta, Y_1, \ldots, Y_N) Y_i^- = \alpha_i(\theta^+, \psi(Y_1), \ldots, \psi(Y_N)) Y_i^- \geq 0.
\]

Therefore we infer from (4.13) that

\[
\frac{1}{2} \frac{d}{dt} \int_\Omega (Y_i^-)^2 dx \leq 0,
\]

which on integrating yields, due to the positivity of the initial data (cf. (2.28)):

\[
Y_i(x,t) \geq 0 \text{ for } t \in [0,T] \text{ and a.e. } x \in \Omega.
\]

Consequently, recalling again the definition (4.1), we now have

\[
\hat{a}_{ij}(Y_1, \ldots, Y_N) = \xi \left( \sum_{\ell=1}^N Y_{\ell} \right) a_{ij}(Y_1, \ldots, Y_N)
\]

so that

\[
\sum_{i=1}^N \hat{F}_i = - \xi \left( \sum_{\ell=1}^N Y_{\ell} \right) \left[ \sum_{i,j=1}^N a_{ij}(Y_1, \ldots, Y_N) \nabla Y_j \right] = 0,
\]

thanks to (2.9).

We aim now to derive (4.12). Let us add the equations (4.3) for \( i = 1, \ldots, N \). By (4.15), the sum of the fluxes vanishes while the property (2.17) still holds for the extended non lineairities \( \omega_i \). Consequently, \( U = \sum_{i=1}^N Y_i \) satisfies:

\[
\frac{\partial U}{\partial \ell} + (v \cdot \nabla) U - \varepsilon \nabla \cdot [\nabla Y^q - 2 \nabla U] = 0.
\]
In view of the boundary conditions for the $Y_i$, we have $U = 1$ on $\Gamma_0$ while, on $\Gamma_h \cup \Gamma_\ell$, by adding the conditions (4.5) and using again (4.15), we see that:

$$\varepsilon|\nabla Y|^q - \frac{\partial U}{\partial \nu} = 0$$

which guarantees that $\frac{\partial U}{\partial \nu} = 0$ on $\Gamma_h \cup \Gamma_\ell$. This gives readily (4.12) since the linear equation (4.16) possesses a unique solution satisfying the above boundary conditions together with $U = 1$ at $t = 0$.

This concludes the proof of Proposition 4.2, since (4.12) together with the positivity of the $Y_i$ provide that $Y_i(x, t) \leq 1$ for $t \in [0, T]$ and a.e. $x \in \Omega$. □

It is worth noting that, since $Y_i(x, t) \geq 0$ and $\sum_{i=1}^{N} Y_i(x, t) = 1$ a.e., we have $\hat{a}_{ij}(Y) = a_{ij}(Y)$ so that (4.3) now reads

$$\frac{\partial Y_i}{\partial t} + (v \cdot \nabla) Y_i - \sum_{j=1}^{N} \nabla \cdot (a_{ij}(Y_1, \ldots, Y_N) \nabla Y_j)$$

$$- \varepsilon \nabla \cdot (|\nabla Y|^q - 2 \nabla Y_i) = \omega_i(\theta, Y_1, \ldots, Y_N).$$

Also, the fluxes in (4.17) are indeed the solutions of the Stefan Maxwell equations (see Theorem 3.2).

4.2. The energy equation.

We aim now to prove Theorem 2.1. The solution of (2.4), (2.22), (2.26) will be obtained by taking the limit $\varepsilon \to 0$ in (4.17). For that purpose we need a priori estimates independent of $\varepsilon$ for the solutions of this problem (we still omit to denote the dependence of $Y_i$ on $\varepsilon$ to make notations simpler).

As mentioned in the introduction, for the original problem (2.4), assuming that the $Y_i$ ($X_i$) do not vanish, the natural Gibbs energy equation is obtained by multiplying equations (2.4) by $\mu_i = \frac{1}{M_i} \log X_i$ and adding for $i = 1, \ldots, N$. More precisely, in view of the boundary conditions, we should multiply (2.4) by

$$\mu_i - \mu_i^u = \frac{1}{M_i}(\log X_i - \log X_i^u),$$

with

$$X_i^u = \frac{Y_i^u}{M_i Y_M}, \quad Y_M^u = \sum_{i=1}^{N} \frac{Y_i^u}{M_i}.$$ 

The $\mu_i$ (resp. $\mu_i^u$) can be expressed in terms of the $Y_j$ (resp. $Y_j^u$) by using the $X - Y$ relations (3.12):

$$\mu_i = \frac{1}{M_i} \log \frac{Y_i}{M_i Y_M} = \frac{1}{M_i} \log \frac{Z_i}{\sum_{j=1}^{N} Z_j} \quad \text{with} \quad Z_i = Y_i/M_i.$$ 

(resp. $Z_i^u = Y_i^u/M_i$).

From a mathematical point of view, since the $Y_i$ might vanish, we introduce a parameter $\eta > 0$, and, instead of $\mu_i$, consider:

$$\mu_i^\eta = \frac{1}{M_i} \log \frac{Z_i^\eta}{\sum_{j=1}^{N} Z_j^\eta}, \quad Z_i^\eta = \frac{Y_i + \eta}{M_i},$$

with a similar definition for $\mu_i^{u, \eta}$. 

We multiply the equations (4.17) by $\mu^\eta_i - \mu^{u,\eta}_i$, integrate over $\Omega$ and add for $i = 1, \ldots, N$. For the term involving the time derivatives, we observe that

\begin{equation}
\mu^\eta_i - \mu^{u,\eta}_i = \frac{\partial}{\partial Y_i} g^\eta(Y_1, \ldots, Y_N),
\end{equation}

where

\begin{equation}
g^\eta(Y_1, \ldots, Y_N) = \sum_{j=1}^{N} \frac{Z_j^\eta}{\sum_{\ell=1}^{N} Z_\ell^\eta} \left[ \log \frac{Z_j^\eta}{\sum_{\ell=1}^{N} Z_\ell^\eta} - \log \frac{Z^{u,\eta}_j}{\sum_{\ell=1}^{N} Z^{u,\eta}_\ell} \right].
\end{equation}

Hence

\begin{equation}
\sum_{i=1}^{N} \left( \frac{\partial Y_i}{\partial t}, \mu^\eta_i - \mu^{u,\eta}_i \right) = \sum_{i=1}^{N} \int_{\Omega} \frac{\partial g^\eta}{\partial Y_i} \frac{\partial Y_i}{\partial t} dx,
\end{equation}

and

\begin{equation}
\sum_{i=1}^{N} < \frac{\partial Y_i}{\partial t}, \mu^\eta_i - \mu^{u,\eta}_i > = \frac{d}{dt} \int_{\Omega} g^\eta(Y_1, \ldots, Y_N) dx.
\end{equation}

Note that $g^\eta$ is bounded independently of $\eta \in [0, 1]$ for bounded values of $Z_j^\eta$ ($0 \leq Z_j^\eta \leq 2/M_j$ in our case). Note also that (4.24) proven as if the $Y_i$ were smooth can be proven by approximation for the actual functions $Y_i$, observing that

\begin{equation}
\frac{\partial Y_i}{\partial t} \in L^q(0, T; (W^{1,q}_0(\Omega))') \quad \text{and} \quad \mu^\eta_i - \mu^{u,\eta}_i \in L^q(0, T; W^{1,q}_0(\Omega)).
\end{equation}

A similar remark applies to several of the following terms.

Next, concerning the contribution of the convective terms to the energy equation, we write

\begin{equation}
\sum_{i=1}^{N} \int_{\Omega} [(v \cdot \nabla) Y_i](\mu^\eta_i - \mu^{u,\eta}_i) = \sum_{j=1}^{N} \int_{\Omega} v_j \frac{\partial}{\partial x_j} g^\eta(Y) dx
\end{equation}

\begin{equation}
= \int_{\partial \Omega} (v \cdot n) g^\eta(Y) d\Gamma - \int_{\Omega} \text{div} \ v g^\eta(Y) dx = \int_{\Gamma_h} \text{div} \ v g^\eta(Y) d\Gamma,
\end{equation}

as $\text{div} \ v = 0, \ g^\eta(Y) = 0$ at $x_n = 0$ and in view of the boundary conditions for $v$.

Performing also some integration by parts in the integrals related to the diffusive terms and nonlinear Laplacian, our energy equation reads

\begin{equation}
\frac{d}{dt} \int_{\Omega} g^\eta(Y) dx + \int_{\Gamma_h} g^\eta(Y) d\Gamma + \sum_{i,j=1}^{N} \int_{\Omega} a_{ij}(Y) \nabla Y_j \cdot \nabla \mu^\eta_i dx
\end{equation}

\begin{equation}
+ \sum_{i=1}^{N} \int_{\Omega} |\nabla Y|^q - 2 \nabla Y_i \cdot \nabla \mu^\eta_i dx = \sum_{i=1}^{N} \int_{\Omega} \omega_i(\theta, Y)(\mu^\eta_i - \mu^{u,\eta}_i) dx.
\end{equation}

We now aim and to pass to the limit $\eta \to 0$ in (4.26). We plan in this way to obtain estimates independent of $\varepsilon$ for the $Y_i = Y_i, \varepsilon$. Note that $\mu^\eta_i$ is singular when $\eta \to 0$ if $Y_i = 0$ but as we will see below this singularity is usually absorbed by other factors.
4.3. Passage to the limit $\eta \to 0$.

We first observe that the right hand-side of (4.26) is bounded from above independently of $\eta \in [0,1]$ and $\varepsilon > 0$. Indeed recalling the decomposition (2.15) of $\omega_i$, we have:

\begin{equation}
\omega_i(\theta, Y)(\mu_i^\eta - \mu_i^{u,\eta}) = \alpha_i(\theta, Y)\mu_i^\eta - \beta_i(\theta, Y)Y_i\mu_i^\eta - \omega_i(\theta, Y)\mu_i^{u,\eta}.
\end{equation}

Here, the assumption (2.16) together with the definition (4.21) of $\mu_i^\eta$ guarantee that $\alpha_i(\theta, Y)\mu_i^\eta \leq 0$ while, by (2.18), $\beta_i$ and $\omega_i$ are bounded functions. Next $\mu_i^\eta$ reads

\begin{equation}
\mu_i^\eta = \frac{1}{M_i} \log \frac{Y_i + \eta}{M_i Y_M^\eta} \quad \text{with} \quad Y_M^\eta = \sum_{j=1}^N Z_j^\eta.
\end{equation}

Since $Y_i \geq 0$ and $\sum_{j=1}^N Y_j = 1$ a.e., the lower bound (3.14) holds true and $Y_M^\eta$ is bounded from below:

\begin{equation}
Y_M^\eta \geq Y_M \geq \frac{1}{M}.
\end{equation}

Consequently the quantities $Y_i\mu_i^\eta$ are bounded independently of $0 < \eta < 1$ and $\varepsilon$ while, since all the $Y_i^u$ are strictly positive, the constants $\mu_i^{u,\eta}$ are also bounded.

Also, recall that $g^\eta(Y)$ given by (4.23) is bounded independently of $\eta \in [0,1]$ and $\varepsilon > 0$. Therefore, coming back to (4.26) that we integrate on $(0,T)$, we conclude that there exists a constant $c_2$ independent of $0 < \eta < 1$ and $\varepsilon$ such that:

\begin{equation}
\sum_{i,j=1}^N \int_0^T \int_\Omega a_{ij}(Y) \nabla Y_j \cdot \nabla \mu_i^\eta dxds + \sum_{i=1}^N \varepsilon \int_0^T \int_\Omega |\nabla Y|^q - 2 \nabla Y_i \cdot \nabla \mu_i^\eta dxds \leq c_2.
\end{equation}

We now aim to take the limit $\eta \to 0$ in the two terms in the right hand-side of (4.29). It follows from (4.28) that

\begin{equation}
\nabla \mu_i^\eta = \frac{1}{M_i} \nabla \frac{Y_i + \eta}{Y_M^\eta} - \frac{1}{M_i} \nabla Y_M^\eta.
\end{equation}

Hence, for the first term in (4.29), we can write:

\begin{equation}
\int_0^T \int_\Omega a_{ij}(Y) \nabla Y_j \cdot \nabla \mu_i^\eta dxds = \int_0^T \int_\Omega \left[ \frac{a_{ij}(Y)}{M_i(Y_i + \eta)} \nabla Y_j \cdot \nabla Y_i - \frac{a_{ij}(Y)}{M_i Y_M^\eta} \nabla Y_j \cdot \nabla Y_M \right] dxds.
\end{equation}

We observe that all the integrands vanish a.e. when $Y_i = 0$ since either $i \neq j$ and, by (2.10), $a_{ij} = 0$, or $i = j$ and $\nabla Y_i$ vanishes (a.e.). Next, we can easily pass to the limit $\eta \to 0$ in the second integral of the right hand-side of (4.31) by using Lebesgue’s theorem since $Y_M^\eta$ is bounded from above and from below by positive constants (independent of $\eta$) and converges pointwise to $Y_M$ as $\eta \to 0$, while the other functions are integrable since $\nabla Y_j \in L^q(0,T; L^q(\Omega))^n$. Hence we obtain

\begin{equation}
\int_0^T \int_\Omega \frac{a_{ij}(Y)}{M_i Y_M^\eta} \nabla Y_j \cdot \nabla Y_M dxds \to \int_0^T \int_\Omega \frac{a_{ij}(Y)}{M_i Y_M^\eta} \nabla Y_j \cdot \nabla Y_M dxds.
\end{equation}

For the first integral in (4.31), we will use the properties (2.10), (2.11) and distinguish the cases $i \neq j$ and $i = j$. If $i \neq j$, in view of (2.10), we observe that:

\begin{equation}
\frac{a_{ij}(Y)}{M_i(Y_i + \eta)} \nabla Y_j \cdot \nabla Y_i = \mathbbm{1}_{\{Y_i > 0\}} \frac{b_{ij}(Y)}{M_i} \frac{Y_i}{Y_i + \eta} \nabla Y_j \cdot \nabla Y_i.
\end{equation}

This quantity converges pointwise to

\begin{equation}
\mathbbm{1}_{\{Y_i > 0\}} \frac{b_{ij}(Y)}{M_i} \nabla Y_j \cdot \nabla Y_i = \mathbbm{1}_{\{Y_i > 0\}} \frac{a_{ij}(Y)}{M_i Y_i} \nabla Y_j \cdot \nabla Y_i.
\end{equation}
and the corresponding integrals converge by Lebesgue’s theorem. Next if \( i = j \), by (2.11),
\[
\frac{a_{ii}(Y)}{M_i(Y_i + \eta)}|\nabla Y_i|^2 = \frac{b_i^0(Y)}{M_i(Y_i + \eta)}|\nabla Y_i|^2 + \frac{b_i^1(Y)}{M_i} \frac{Y_i}{Y_i + \eta} |\nabla Y_i|^2.
\]
Similarly to above, we have
\[
\frac{b_i^1(Y)}{M_i} \frac{Y_i}{Y_i + \eta} |\nabla Y_i|^2 \to 1_{\{Y_i > 0\}} \frac{b_i^0(Y)}{M_i} |\nabla Y_i|^2,
\]
hence the convergence of the integrals. For the terms involving \( b_i^0 \), we observe that \( b_i^0(Y) \geq 0 \) so that we can pass to the lower limit by Fatou’s Lemma and obtain:
\[
\int_0^T \int_\Omega 1_{\{Y_i > 0\}} \frac{b_i^0(Y)}{M_i} \frac{Y_i}{Y_i + \eta} |\nabla Y_i|^2 \, dxds = \liminf_{\eta \to 0} \int_0^T \int_\Omega 1_{\{Y_i > 0\}} \frac{b_i^0(Y)}{M_i} \frac{Y_i}{Y_i + \eta} |\nabla Y_i|^2 \, dxds.
\]
In the context of the final a priori estimates below (collected estimates), (4.32) implies that its left hand-side is indeed integrable.

Using again (4.30), the second term in (4.29) reads:
\[
\sum_{i=1}^N \varepsilon \int_0^T \int_\Omega |\nabla Y|^q |\nabla Y_i| \cdot \nabla \mu_i \, dxds = \sum_{i=1}^N \varepsilon \int_0^T \int_\Omega |\nabla Y|^q |\nabla Y_i|^2 M_i(Y_i + \eta) \, dxds - \varepsilon \int_0^T \int_\Omega |\nabla Y|^q \frac{|\nabla Y_M|^2}{Y_M^2} \, dxds.
\]
We can easily pass to the limit \( \eta \to 0 \) by using Lebesgue’s theorem in the second term. Concerning the first one, the integrand is positive, so we can take the lower limit using Fatou’s Lemma so that:
\[
\sum_{i=1}^N \varepsilon \int_0^T \int_\Omega |\nabla Y|^q |\nabla Y_i|^2 1_{\{Y_i > 0\}} \frac{1}{M_i} \frac{|\nabla Y_i|^2}{Y_i} \, dxds
\leq \liminf_{\eta \to 0} \sum_{i=1}^N \varepsilon \int_0^T \int_\Omega |\nabla Y|^q |\nabla Y_i|^2 1_{\{Y_i > 0\}} \frac{|\nabla Y_i|^2}{M_i(Y_i + \eta)} \, dxds.
\]
As for (4.32), this eventually implies that the left hand side of (4.34) is integrable.

By collecting all the results above we can pass to the lower limit in (4.29) as \( \eta \to 0 \) and we obtain that:
\[
\int_0^T \int_\Omega \sum_{i,j=1}^N 1_{\{Y_i > 0\}} a_{ij}(Y) \nabla Y_i \cdot \nabla \mu_j \, dxds + \varepsilon \int_0^T \int_\Omega |\nabla Y|^q \left\{ \sum_{i=1}^N \frac{|\nabla Y_i|^2}{M_i Y_i} 1_{\{Y_i > 0\}} - \frac{|\nabla Y_M|^2}{Y_M} \right\} \, dxds \leq c_2.
\]

4.4. Passage to the limit \( \varepsilon \to 0 \).
We first derive from (4.35) some estimates of the \( Y_i = Y_i, \varepsilon \) that are independent of \( \varepsilon \). Recalling (2.8), we observe that the first term in (4.35) is equal to
\[
- \sum_{i=1}^N \int_0^T \int_\Omega F_i \cdot \nabla \mu_i 1_{\{Y_i > 0\}} \, dxds,
\]
and thanks to (2.12) it is bounded from below by
\[ c_1 \int_0^T \int_\Omega |\nabla Y|^2 \, dx \, ds. \]

Also we observe that the second term in (4.35) is positive because
\[
\frac{|\nabla Y_M|^2}{Y_M^2} = \frac{1}{Y_M} \left| \sum_{j=1}^N \frac{\nabla Y_j}{M_j} \mathbb{1}_{\{Y_j > 0\}} \right|^2 \\
\leq \frac{1}{Y_M} \left( \sum_{j=1}^N \frac{|\nabla Y_j|^2}{M_j Y_j} \mathbb{1}_{\{Y_j > 0\}} \right) \left( \sum_{j=1}^N \frac{Y_j}{M_j} \right) \\
\leq \sum_{j=1}^N \frac{|\nabla Y_j|^2}{M_j Y_j} \mathbb{1}_{\{Y_j > 0\}}.
\]

With this (4.35) yields
\[
(4.36) \quad c_1 \int_0^T \int_\Omega |\nabla Y|^2 \, dx \, ds \leq c_2,
\]
where \(c_1\) and \(c_2\) are independent of \(\varepsilon\), so that:
\[
(4.37) \quad \int_0^T \int_\Omega |\nabla Y|^2 \, dx \, ds \text{ is bounded independently of } \varepsilon.
\]

Going back to (4.10), (4.37) together with (4.11) guarantee that
\[
(4.38) \quad \varepsilon \int_0^T \int_\Omega |\nabla Y|^q \, dx \, ds \text{ is bounded independently of } \varepsilon.
\]

Thanks to the estimates (4.8), (4.37) and (4.38), we can take the limit \(\varepsilon \to 0\) in (4.17) and obtain a weak solution of (2.4). The details are standard. This concludes the proof of Theorem 2.1.

5. The Full System

In this section, we investigate problem (2.1)-(2.4) and aim to prove Theorem 2.2. The \(Y\)– system is now coupled with the equations for \(v\) and \(\theta\). Clearly, in comparison with our study in Section 4, the main new point is to derive estimates like (2.30), (2.31) for \(v\) and \(\theta\). As in Section 4, we derive such estimates for an appropriate modified problem, and then we take the limit \(\varepsilon \to 0\).

The \(Y\)– equations (2.4) are modified as in Section 4 by considering (4.3). Now, this system is coupled with
\[
(5.1) \quad \frac{\partial v}{\partial t} + (v \cdot \nabla) v - Pr \Delta v + \nabla p = e_n \sigma \theta,
\]
\[
(5.2) \quad \text{div } v = 0,
\]
\[
(5.3) \quad \frac{\partial \theta}{\partial t} + (v \cdot \nabla) \theta - \Delta \theta = -\sum_{i=1}^N h_i \omega_i (\theta, Y_1, \ldots, Y_N).
\]

As before, we show the existence of a solution of (5.1)-(5.3), (4.3) (together with the appropriate initial and boundary conditions) thanks to the methods of compactness and monotonicity. The useful a priori estimates derived hereafter are based on the fact that
the \( \omega_i \) are bounded independently of \( Y \) and \( \theta \), thanks to (4.2). We first multiply (5.3) by \( \theta \) and integrate over \( \Omega \). This provides

\[
\frac{1}{2} \frac{d}{dt} \int_{\Omega} \theta^2 dx + \frac{1}{2} \int_{\Gamma_h} \theta^2 d\Gamma + \int_{\Omega} |\nabla \theta|^2 dx = - \int_{\Omega} \left( \sum_{i=1}^{N} h_i \omega_i(\theta, Y) \right) \theta dx \\
\leq \text{ (due to (4.2))} \\
\leq K_2 \left( \sum_{i=1}^{N} h_i \right) \int_{\Omega} |\theta| dx,
\]

which yields readily that

\[
\text{(5.4)} \quad \theta \text{ is bounded in } L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)).
\]

Now, the right-hand side of (5.1) is bounded in \( L^\infty(0, T, L^2(\Omega)) \). Classical estimates for the two and three dimensional Navier-Stokes equations (see e.g. [Tem77]) provide that

\[
\text{(5.5)} \quad v \text{ is bounded in } L^\infty(0, T, L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)).
\]

In particular, the estimates corresponding to (2.30) and (2.31) have now been derived for \( v \) and \( \theta \). We can then proceed as in the proof of Proposition 4.2 and show that

\[
\text{(5.6)} \quad Y \text{ is bounded in } L^\infty(0, T, L^2(\Omega)) \cap L^q(0, T; W^{1,q}(\Omega)).
\]

It follows easily from (5.4)-(5.6) that the system consisting of (4.3) and (5.1)-(5.3) supplemented with the boundary conditions (2.20), (2.21), (2.22), (4.5) and the initial conditions (2.25), (2.26) possesses a solution \((v, \theta, Y)\). Also, (4.11), (4.12) hold for the same reasons as before. Furthermore we have

\[
\text{(5.7)} \quad \theta(x, t) \geq 0 \text{ for } t \in [0, T] \text{ and a.e. } x \in \Omega.
\]

Indeed, multiplying (5.3) by \( -\theta^- = \min(0, \theta) \) and integrating over \( \Omega \), we obtain

\[
\frac{1}{2} \frac{d}{dt} \int_{\Omega} (\theta^-)^2 dx + \frac{1}{2} \int_{\Gamma_h} (\theta^-)^2 d\Gamma + \int_{\Omega} |\nabla \theta^-|^2 dx = \int_{\Omega} \left( \sum_{i=1}^{N} h_i \omega_i(\theta, Y) \right) \theta^- dx.
\]

(5.8)

Due to the definition (2.29) of \( \omega_i \) and (2.19), at each point \((x, t)\) such that \( \theta(x, t) \leq 0 \), we have

\[
\sum_{i=1}^{N} h_i \omega_i(\theta, Y) = \sum_{i=1}^{N} h_i \omega_i(0, Y) \leq 0,
\]

and therefore

\[
\int_{\Omega} \left( \sum_{i=1}^{N} h_i \omega_i(\theta, Y) \right) \theta^- dx \leq 0.
\]

(5.9)

Combining (5.9) with (5.8) enables us to show that

\[
\frac{d}{dt} \int_{\Omega} (\theta^-)^2 dx \leq 0,
\]

and thus to obtain (5.7) since \( \theta_0(x) \geq 0 \) for almost every \( x \in \Omega \).

The modified system (5.1)-(5.3), (4.3), (4.5) depends on a parameter \( \varepsilon > 0 \) (in (4.3) and (4.5)) and as in Section 4 we need to take the limit \( \varepsilon \to 0 \). The estimates (5.4) and (5.5) are independent of \( \varepsilon \) while \( Y \) can be estimated independently of \( \varepsilon \) exactly as in Section 4. Based on these estimates it is easy to see that we can take the limit \( \varepsilon \to 0 \) in (5.1)-(5.3), (4.3), (4.5) and obtain a weak solution of (2.1)-(2.4). The passage to the limit in the \( Y\)–
equations is done as in Section 4; the passage to the limit in the $v$ and $\theta$ equations is standard. The details are left to the reader.

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