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Fully Nonlinear Multispecies Reaction-Diffusion Equations

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Abstract—We consider combustion problems in the presence of complex chemistry leading to fully nonlinear multispecies reaction-diffusion equations. We establish results of existence and uniqueness of solution and maximum principle i.e., positivity of the mass fractions, which relies on specific properties of the models.

Keywords—Nonlinear partial differential equations, Combustion, Reaction diffusion equations, Stefan-Maxwell equations.

1. INTRODUCTION

We continue previous work on the equations of combustion in the presence of complex chemistry. In [1], we considered a model of laminar premixed flame in which the binary transport coefficients were constants equal to one another, and hence, the fluxes were proportional to the gradients of the mass fractions of the species. Here we remove this simplifying hypothesis and assume that the fluxes are given by the Stefan Maxwell equations. In this case, the concentration equations become fully nonlinear with nonlinearity involving the highest derivatives.

In this note, we emphasize the reaction-diffusion part of the complex chemistry problem; the coupling with the heat equation and fluid motion will be developed in more details in [2]. We discuss the derivation of the concentration equations by solution of the Stefan Maxwell equations and develop their mathematical theory including existence and uniqueness of solutions and maximum principle. Applications to atmosphere and pollution problems will be discussed elsewhere.

We consider a multi-component premixed gas flame propagating in a bounded channel $\Omega \subset \mathbb{R}^n, n = 2$ or 3. Assuming that the fluid is incompressible, with nondimensional density equal to one, the equations for the reactive flow read

$$\frac{\partial Y_i}{\partial t} + (v \cdot \nabla) Y_i + \nabla \cdot F_i = \omega_i, \qquad 1 \le i \le N, \tag{1.1}$$

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$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v - \mathrm{Re}\,\Delta v + \nabla p = 0, \qquad \operatorname{div} v = 0, \tag{1.2}$$

$$\frac{\partial \theta}{\partial t} + (v \cdot \nabla)\theta - \mathrm{Pr}\,\Delta \theta = -\sum_{i=1}^{N} h_i \omega_i. \tag{1.3}$$

The unknowns which are in nondimensional form are the velocity $v = (v_1, v_2)$ or (v_1, v_2, v_3), the pressure p, the temperature θ and the mass fraction Y_i of the N species involved in the chemical reaction; $\mathrm{Re} > 0$ and $\mathrm{Pr} > 0$ are the Reynolds and Prandtl numbers; h_i is the enthalpy of the i^{th} species and ω_i is the net production/removal rate of the i^{th} species [3].

On physical grounds, the following relations must prevail at all time

$$0 \le Y_i \le 1, \quad 1 \le i \le N, \quad \sum_{i=1}^{N} Y_i = 1, \tag{1.4}$$

$$\sum_{i=1}^{N} \omega_i = 0. \tag{1.5}$$

The fluxes F_i in (1.1) read

$$F_i = Y_i V_i, \tag{1.6}$$

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

$$\sum_{i=1}^{N} F_i = \sum_{i=1}^{N} Y_i V_i = 0. \tag{1.7}$$

The V_i, and therefore the F_i, are given by resolution of the Stefan-Maxwell equations (cf. [4]) which we discuss in the following section. They give the F_i as linear-functions of $\nabla Y_1, \dots, \nabla Y_N$ with coefficients involving rational functions of $Y_1, \dots, Y_N$.

Note that the equations for the hydrodynamical unknowns (v, p) are decoupled from the temperature and concentrations. In fact, we will study in a first step the equation (1.1) assuming that v, p and θ are known; then we will show how to couple the whole system.

2. THE STEFAN-MAXWELL EQUATIONS

These equations allowing the determination of the F_i read

$$\nabla X_i = \sum_{\substack{j=1 \\ j \ne i}}^{N} d_{ij} X_i X_j (V_j - V_i), \qquad i = 1, \dots, N, \tag{2.1}$$

where $d_{ij} = 1/D_{ij}, D_{ij} = D_{ji} > 0$ is the binary diffusion coefficient for species i and j. The mole fraction X_i of species i is related to the mass fractions by the formula

$$X_i = \frac{Y_i}{M_i Y_M}, \quad Y_M X_M = 1, \tag{2.2}$$

$$Y_M = \sum_{j=1}^{N} \frac{Y_j}{M_j}, \qquad X_M = \sum_{j=1}^{N} M_j X_j, \tag{2.3}$$

where $M_i > 0$ is the molecular mass; hence we have also

$$0 \le X_i \le 1, \quad 1 \le i \le N, \quad \sum_{i=1}^{N} X_i = 1. \tag{2.4}$$

We see the equations (2.1) as a linear system for the V_i, which gives in principle the V_i as linear functions of the ∇X_j with coefficients involving the X_j. When the X_j are expressed in terms of the Y_j by (2.2) and (2.3), (2.1) gives in principle the V_i as linear functions of the ∇Y_j with coefficients involving rational functions of the Y_j.

With obvious notations we write the linear system (2.1) in the form

$$B(Y)V = -\nabla X, \tag{2.5}$$

$V = (V_1, \dots, V_N), \nabla X = (\nabla X_1, \dots, \nabla X_N)$, and we observe that

$$(B(Y)V, V) = \sum_{1 \le i < j \le N} \frac{d_{ij}}{M_i M_j} \frac{Y_i Y_j}{Y_M^2} |V_i - V_j|^2 \ge 0.$$

Hence, if $Y_i > 0, \forall i$, the matrix $B(Y)$ has rank $N - 1$ and the solution of (2.5) is unique thanks to (1.7).

When some of the Y_i are allowed to vanish (while (1.4) is satisfied), we cannot resolve anymore the system (2.5). However an involved study of this system conducted in [2] shows that one can determine in a unique way the F_i as rational functions of the Y_j and ∇Y_j. We now list the properties of these functions proven in [2] and which are the basis for the study conducted in Sections 3 and 4 below:

$$\begin{aligned} &F_i = -\sum_{j=1}^{N} a_{ij}(Y_1, \dots, Y_N)\nabla Y_j, \qquad 1 \le i \le N, \\ &\sum_{i=1}^{N} F_i = 0. \end{aligned} \tag{2.6}$$

The functions a_{ij} are continuous functions from $[0,1]^N$ into $\mathbb{R}$ such that

$$\begin{aligned} &a_{ij}(Y_1, \dots Y_N) = Y_i b_{ij}(Y_1, \dots, Y_N) \text{ for } i \ne j \text{ and } 0 \le Y_k \le 1, \\ &\text{where } b_{ij} : [0,1]^N \to \mathbb{R} \text{ is continuous,} \end{aligned} \tag{2.7}$$

$$\begin{aligned} &a_{ii}(Y_i, \dots, Y_N) = b_{ii}^0(Y_1, \dots, Y_N) + Y_i b_{ii}^1(Y_i, \dots, Y_N) \text{ for } 0 \le Y_k \le 1, \\ &\text{where } b_{ii}^0(Y) \ge 0 \text{ and } b_{ii}^j : [0,1]^N \to \mathbb{R} \text{ is continuous, } j = 0, 1. \end{aligned} \tag{2.8}$$

REMARK 2.1. The computation of the diffusion coefficients by different methods appears in [5].

3. THE REACTION DIFFUSION EQUATIONS

The chemical rates ω_i are assumed to be of the form

$$\omega_i = \omega_i(\theta, Y_1, \dots, Y_N) = \alpha_i(\theta, Y_1, \dots, Y_N) - Y_i \beta_i(\theta, Y_1, \dots, Y_N). \tag{3.1}$$

The functions α_i and β_i are defined for $\theta \ge 0, 0 \le Y \le 1$ and are assumed to be continuous on $[0, \infty) \times [0,1]^N$ and such that

$$\alpha_i(\theta, Y_1, \dots, Y_N) \ge 0, \quad \beta_i(\theta, Y_1, \dots Y_n) \ge 0, \qquad \text{for } \theta \ge 0, \quad 0 \le Y_j \le 1, \tag{3.2}$$

$$\sum_{i=1}^{N} h_i \omega_i(\theta, Y_1, \dots Y_N) \le 0, \qquad \text{for } 0 \le Y_j \le 1, \tag{3.3}$$

$$\sum_{i=1}^{N} \omega_i(\theta, Y_1, \dots, Y_N) = 0, \qquad \text{for } \theta \ge 0, \quad 0 \le Y_j \le 1, \tag{3.4}$$

$$\omega_i \text{ is bounded on } [0, \infty) \times [0,1]^N. \tag{3.5}$$

The domain Ω in which the flame propagates is the channel $\Omega = (0, \ell) \times (0, h)$ for $n = 2$ and $\Omega = (0, \ell) \times (0, L) \times (0, h)$ for $n = 3$. We assume that the flame propagates in the x_n direction, the premixed reacting species entering from below. Hence,

$$\begin{aligned} &Y_i = Y_i^u \text{ at } x_n = 0, \quad \frac{\partial Y_i}{\partial x_n} = 0 \text{ at } x_n = h, \\ &\frac{\partial Y_i}{\partial \nu} = 0 \text{ at } x_1 = 0,\ \ell \text{ (and } x_2 = 0, L \text{ if } n = 3) \end{aligned} \tag{3.6}$$

where $Y_i^u > 0, \sum_{i=1}^N Y_i^u = 1$.

Here we assume that v and θ are given satisfying

$$v \in L^\infty\left(0, T; L^2(\Omega)^N\right) \cap L^2\left(0, T; H^1(\Omega)^N\right), \tag{3.7}$$

$$\theta \in L^\infty\left(0, T; L^2(\Omega)\right) \cap L^2\left(0, T; H^1(\Omega)\right), \qquad \theta(x, t) \geq 0 \text{ a.e.} \tag{3.8}$$

We assume also that v and θ satisfy the boundary conditions of the full problem (see (4.1) and (4.2) below). The initial condition reads

$$Y_i(x, 0) = Y_{i0}(x), \quad Y_{i0}(x) \geq 0, \quad \sum_{i=1}^N Y_{i0}(x) = 1, \text{ a.e.} \tag{3.9}$$

The result is the following theorem.

THEOREM 3.1. *For v and θ given as above, equations (1.1) with (1.6), (1.7), (2.1), (3.6) and (3.9) possess a unique solution $Y_1, \dots, Y_N$ such that*

$$\begin{aligned} &Y_i \in L^2\left(0, T; H^1(\Omega)^N\right), \qquad \forall T > 0, \\ &Y_i(x, t) \geq 0, \quad \sum_{i=1}^N Y_i(x, t) = 1, \qquad \text{a.e. } x \in \Omega, \quad t > 0, \quad 1 \leq i \leq N. \end{aligned} \tag{3.10}$$

The proof of Theorem 3.1 will be given in [2]. It consists in approximating equations (1.1) by a set of regularized equations for which (1.4) is not required. We prove (1.4) thanks to (3.7) and to the properties of the regularized equations, and we pass to the limit.

4. THE FULL EQUATIONS

We now consider the full equations (1.1), (1.2), (1.3). The boundary conditions for v and θ are

$$\begin{aligned} &v_i = 0, \qquad 1 \leq i \leq n-1, \quad v_n = 1 \text{ at } x_n = 0, h, \\ &v_i = 0, \qquad 1 \leq i \leq n-1, \quad \frac{\partial v_n}{\partial \nu} = 0 \text{ at } x_1 = 0, \ell \text{ (and } x_2 = 0, L \text{ if } n = 3), \end{aligned} \tag{4.1}$$

$$\begin{aligned} &\theta = 0 \text{ at } x_n = 0, \qquad \frac{\partial \theta}{\partial x_n} = 0 \text{ at } x_n = h, \\ &\frac{\partial \theta}{\partial \nu} = 0 \text{ at } x_1 = 0,\ \ell \text{ (and } x_2 = 0, L \text{ if } n = 3). \end{aligned} \tag{4.2}$$

The initial data for v and θ are given

$$v(x, 0) = v_0(x), \quad \theta(x, 0) = \mathrm{O}_0(x) \geq 0, \qquad \text{a.e. } x \in \Omega. \tag{4.3}$$

THEOREM 4.1. *For v_0, θ_0, Y_0 given as above, equations (1.1), (1.2), (1.3) and (2.1) supplemented by (3.5), (3.9), (4.1)–(4.3), possess a unique solution $\theta, v, Y_1, \dots, Y_N$ satisfying (3.7), (3.8), (3.10), for every $T > 0$ if $n = 2$.*

If $n = 3$, the solution exists but is not known to be unique.[1]

The proof of Theorem 4.1 is based on Theorem 3.1, using a fixed point method. For (v, θ) given, we solve equations (1.1) using Theorem 3.1; we then solve equations (1.2) and (1.3) with these values of $Y_1, \dots, Y_N$, and we obtain $(\tilde{v}, \tilde{\theta}) = \mathcal{T}(v, \theta)$. We then show that $\mathcal{T}$ possesses a fixed point; see [2] for more details.

[1]We meet here the usual difficulties related to the Navier-Stokes equations in space dimension 3, see e.g., [6].

REFERENCES

1. O. Manley, M. Marion and R. Temam, Equations of combustion in the presence of complex chemistry, *Indiana Univ. Math. J.* **42**, 941–967, (1993).
2. O. Manley, M. Marion and R. Temam, Equations of combustion with complex transport coefficients, (in preparation).
3. F.A. Williams, *Combustion Theory*, Second Edition, Benjamin Cummings, Menlo Park, CA, (1985).
4. F.R. Steward, *Radiative Heat Transfer Associated with Fire Problems*, Part IV of *Heat Transfer in Fires: Thermophysics, social aspects, economic impact*, (Edited by P.L. Blackshear), Scripta Book 6, pp. 273-486, Wiley, New York, (1974).
5. A. Ern, *Théorie mathématique et numérique pour l'évaluation des coefficients de transport dans les mélanges gazeux polyatomiques*, Thèse, Ecole Polytechnique, Paris, (1994).
6. R. Temam, *Navier-Stokes Equations*, 3^{rd} Revised Edition, Studies in Mathematics and its Applications 2, North-Holland, (1984).