ECOLE POLYTECHNIQUE

CENTRE DE MATHÉMATIQUES APPLIQUÉES

UMR CNRS 7641

91128 PALAISEAU CEDEX (FRANCE). Tél: 01 69 33 46 00. Fax: 01 69 33 46 46
http://www.cmap.polytechnique.fr/

MULTICOMPONENT FLOW MODELING

Vincent Giovangigli

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Vincent GIOVANGIGLI
CMAP, CNRS, Ecole Polytechnique,
91128 Palaiseau cedex, FRANCE
vincent.giovangigli@polytechnique.fr

Abstract

We first present multicomponent flow models derived from the kinetic theory of gases. We then investigate the symmetric hyperbolic-parabolic structure of the resulting system of partial differential equations and discuss the Cauchy problem for smooth solutions. We also address the existence of deflagration waves also termed anchored waves. We further indicate related models which have a similar hyperbolic-parabolic structure, notably the Saint-Venant system with a temperature equation as well as the equations governing chemical equilibrium flows. We next investigate multicomponent ionized and magnetized flow models with anisotropic transport fluxes which have a different mathematical structure. We finally discuss numerical algorithms specifically devoted to complex chemistry flows, in particular the evaluation of multicomponent transport properties, as well as the impact of multicomponent transport.

1 Introduction

Multicomponent reactive flows with complex chemistry and detailed transport phenomena arise in various engineering applications such as atmospheric reentry [1, 2], crystal growth [3, 4], and combustion [5, 6]. This is a strong motivation for investigating the corresponding governing equations and analyzing their mathematical structure and properties [7].

We first present the governing equations for multicomponent reactive flows in Section 2. These equations are derived from the kinetic theory of polyatomic reactive gas mixtures [7, 8, 9, 10, 11, 12, 13]. In particular, many symmetry properties of the corresponding fluid equations are direct consequences of symmetry properties associated with the Boltzmann collision operator [7].

We next investigate in Section 3 the mathematical structure of the resulting system of partial differential equations and the Cauchy problem [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]. We discuss symmetrizability properties and present global existence theorems around constant equilibrium states as well as asymptotic stability and decay estimates [20]. The method of proof relies on the normal form of the governing equations, on entropic estimates, and on the local dissipativity properties of the linearized equations [15, 20].

We then address the anchored wave problem with complex chemistry and detailed transport in Section 4. Traveling waves in inert or reactive flows can indeed be classified into deflagration and detonation waves. In the context of combustion, weak deflagration waves correspond to plane laminar flames [32, 33, 34, 35, 36]. We investigate the anchored flame model using entropic estimates and the Leray–Schauder topological degree theory [36].

We further discuss in Section 5 various flows whose governing equations share a similar structure with that of multicomponent reactive flows investigated in Section 3. We address in particular the Saint-Venant system [37, 38, 39, 40, 42] with a temperature equation [43] and the equations governing chemical equilibrium flows [7, 44, 45, 46, 47, 48].

The equations governing multicomponent ionized and magnetized mixtures are then investigated in Section 6. These equations are derived from the kinetic theory of weakly ionized plasmas and the corresponding transport fluxes are non isotropic in strong magnetic fields [49, 50, 51, 52, 53]. The resulting mathematical structure is notably more complex than that investigated in Section 3. A new definition of symmetrizability is introduced and local existence is obtained thanks to these partial symmetrization results [51]. This is in constrast with the situation of ambipolar plasmas whose structure is similar to that of isotropic multicomponent flows [24].

We finally discuss in Section 7 the numerical simulation of multicomponent flows with complex chemistry and detailed transport [54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64]. We notably address the mathematical structure of the transport linear systems and fast accurate evaluation of the transport coefficients [65, 66, 67, 68, 69, 70, 71]. We also present a typical numerical simulation of a complex chemistry Bunsen laminar flames [5, 72, 73, 74] and discuss the impact of multicomponent transport [75, 76, 77, 78, 79, 80] as well as possible extensions [81, 82, 83, 84, 85, 86, 87, 88].

2 Multicomponent reactive flow models

The equations governing multicomponent reactive flows are derived form the kinetic theory of polyatomic reactive gas mixtures [7, 8, 9, 10, 11, 12, 13]. These equations can be split between conservation equations, thermochemistry, and transport fluxes.

2.1 Conservation equations

The equations for conservation of species mass, momentum and energy can be written in the form [7]

$$\partial_t \rho_k + \boldsymbol{\partial}_x \boldsymbol{\cdot} (\rho_k \boldsymbol{v}) + \boldsymbol{\partial}_x \boldsymbol{\cdot} \boldsymbol{\mathcal{F}}_k = m_k \omega_k, \qquad k \in S, \tag{2.1}$$

$$\partial_t (\rho \boldsymbol{v}) + \boldsymbol{\partial}_x \boldsymbol{\cdot} (\rho \boldsymbol{v} \otimes \boldsymbol{v} + p \boldsymbol{I}) + \boldsymbol{\partial}_x \boldsymbol{\cdot} \boldsymbol{\Pi} = \rho \boldsymbol{g}, \tag{2.2}$$

$$\partial_t (\mathcal{E} + \tfrac{1}{2} \rho \boldsymbol{v} \boldsymbol{\cdot} \boldsymbol{v}) + \boldsymbol{\partial}_x \boldsymbol{\cdot} \big((\mathcal{E} + \tfrac{1}{2} \rho \boldsymbol{v} \boldsymbol{\cdot} \boldsymbol{v} + p) \boldsymbol{v} \big) + \boldsymbol{\partial}_x \boldsymbol{\cdot} (\boldsymbol{Q} + \boldsymbol{\Pi} \boldsymbol{\cdot} \boldsymbol{v}) = \rho \boldsymbol{v} \boldsymbol{\cdot} \boldsymbol{g}, \tag{2.3}$$

where ∂_t denotes the time derivative, $\boldsymbol{\partial}_x$ the space derivative operator, ρ_k the mass density of the kth species, $\boldsymbol{v}$ the mass average flow velocity, $\boldsymbol{\mathcal{F}}_k$ the diffusion flux of the kth species, m_k the molar mass of the kth species, ω_k the molar production rate of the kth species, $S = \{1, \dots, n\}$ the set of species indices, $n \geqslant 1$ the number of species, $\rho = \sum_{k \in S} \rho_k$ the total mass density, p the pressure, $\boldsymbol{\Pi}$ the viscous tensor, $\boldsymbol{g}$ the gravity, $\mathcal{E}$ the internal energy per unit volume and $\boldsymbol{Q}$ the heat flux. These equations have to be completed by the relations expressing the thermodynamic properties like p and $\mathcal{E}$, the chemical production rates ω_k, $k \in S$, and the transport fluxes $\boldsymbol{\Pi}$, $\boldsymbol{\mathcal{F}}_k$, $k \in S$, and $\boldsymbol{Q}$.

2.2 Thermochemistry

Thermodynamics obtained in the framework of the kinetic theory of gases is valid out of equilibrium and has, therefore, a wider range of validity than classical thermodynamics introduced for stationary homogeneous equilibrium states. The internal energy per unit volume $\mathcal{E}$ and the pressure p can be written in terms of the state variables $T, \rho_1, \dots, \rho_n$ as

$$\mathcal{E}(T, \rho_1, \dots, \rho_n) = \sum_{k \in S} \rho_k e_k(T), \qquad p(T, \rho_1, \dots, \rho_n) = \sum_{k \in S} R_{\mathrm{g}} T \frac{\rho_k}{m_k},$$

where T is the absolute temperature, e_k the internal energy per unit mass of the kth species, and R_{g} the gas constant. The internal energy e_k of the kth species is given by

$$e_k(T) = e_k^{\mathrm{st}} + \int_{T^{\mathrm{st}}}^{T} c_{vk}(\tau)\, d\tau, \qquad k \in S,$$

where e_k^{st} is the standard formation energy of the kth species at the standard temperature T^{st} and c_{vk} the constant volume specific heat of the kth species. It is also possible to use other variables than the partial densities ρ_k, $k \in S$, to describe the mixture as for instance the species mass fractions Y_k, $k \in S$, partial pressures p_k, $k \in S$, or mole fractions X_k, $k \in S$, given by

$$Y_k = \frac{\rho_k}{\rho}, \qquad p_k = \frac{\rho_k R_{\mathrm{g}} T}{m_k}, \qquad X_k = \frac{p_k}{p}, \qquad k \in S,$$

and a particular choice usually depends on the application under consideration. The (physical) entropy per unit volume $\mathcal{S}$ can be written in the form

$$\mathcal{S}(T, \rho_1, \dots, \rho_n) = \sum_{k \in S} \rho_k s_k(T, \rho_k),$$

where s_k is the entropy per unit mass of the kth species. This quantity is in the form

$$s_k(T,\rho_k) = s_k^{\mathrm{st}} + \int_{T^{\mathrm{st}}}^{T} \frac{c_{vk}(T')}{T'}\, dT' - \frac{R_{\mathrm{g}}}{m_k} \log\left(\frac{\rho_k}{\gamma^{\mathrm{st}} m_k}\right), \qquad k \in S,$$

where s_k^{st} is the formation entropy of the kth species at the standard temperature T^{st} and standard pressure $p^{\mathrm{st}} = p^{\mathrm{atm}}$ and $\gamma^{\mathrm{st}} = p^{\mathrm{st}}/R_{\mathrm{g}}T^{\mathrm{st}}$ is the standard concentration. Similarly, one can introduce the mixture enthalpy $\mathcal{H} = \sum_{k\in S} \rho_k h_k(T)$ with $h_k(T) = e_k(T) + R_{\mathrm{g}}T/m_k$, $k \in S$, and the mixture Gibbs function $\mathcal{G} = \sum_{k\in S} \rho_k g_k(T,\rho_k)$, with $g_k(T,\rho_k) = h_k(T) - T s_k(T,\rho_k)$, $k \in S$.

We further assume that there are chemical reactions between the species and we consider a system of $n^{\mathrm{r}} \geqslant 1$ elementary reactions for $n \geqslant 1$ species which can be written formally

$$\sum_{k\in S} \nu_{ki}^{\mathrm{f}}\, \mathfrak{M}_k \rightleftarrows \sum_{k\in S} \nu_{ki}^{\mathrm{b}}\, \mathfrak{M}_k, \qquad i \in \mathfrak{R},$$

where $\mathfrak{M}_k$ is the chemical symbol of the kth species, ν_{ki}^{f} and ν_{ki}^{b} the forward and backward stoichiometric coefficients of the kth species in the ith reaction, $\mathfrak{R} = \{1,\ldots,n^{\mathrm{r}}\}$ the set of reaction indices, and $\nu_{ki} = \nu_{ki}^{\mathrm{b}} - \nu_{ki}^{\mathrm{f}}$ the overall stoichiometric coefficients. A typical chemical reaction mechanism for the combustion of hydrogen in air is presented in Section 7.

The molar production rates that we consider are the Maxwellian production rates obtained from the kinetic theory [7, 13] when the chemical characteristic times are larger than the mean free times of the molecules and the characteristic times of internal energy relaxation. These rates ω_k, $k \in S$, are compatible with the law of mass action and are in the form

$$\omega_k = \sum_{i=1}^{m} (\nu_{ki}^{\mathrm{b}} - \nu_{ki}^{\mathrm{f}}) \left(\mathcal{K}_i^{\mathrm{f}} \prod_{l\in S} \Big(\frac{\rho_l}{m_l}\Big)^{\nu_{li}^{\mathrm{f}}} - \mathcal{K}_i^{\mathrm{b}} \prod_{l\in S} \Big(\frac{\rho_l}{m_l}\Big)^{\nu_{li}^{\mathrm{b}}} \right), \qquad k \in S,$$

where $\mathcal{K}_i^{\mathrm{f}}$ and $\mathcal{K}_i^{\mathrm{b}}$ are the forward and backward rate constants of the ith reaction, respectively. The reaction constants $\mathcal{K}_i^{\mathrm{f}}$ and $\mathcal{K}_i^{\mathrm{b}}$ are functions of temperature and are Maxwellian averaged values of molecular chemical transition probabilities [13]. In particular, forward and backward chemical transition probabilities are always proportional—as are nonreactive cross sections in any Boltzmann equation—and this implies the reciprocity relations [7, 13]

$$\mathcal{K}_i^{\mathrm{e}}(T) = \frac{\mathcal{K}_i^{\mathrm{f}}(T)}{\mathcal{K}_i^{\mathrm{b}}(T)}, \qquad \log \mathcal{K}_i^{\mathrm{e}}(T) = -\sum_{k\in S} \frac{\nu_{ki} m_k}{R_{\mathrm{g}} T} g_k(T, m_k), \qquad i \in \mathfrak{R},$$

where $\mathcal{K}_i^{\mathrm{e}}(T)$ is the equilibrium constant of the ith reaction. On the other hand, the forward reaction constants $\mathcal{K}_i^{\mathrm{f}}$, $i \in \mathfrak{R}$, are usually evaluated with Arrhenius law

$$\mathcal{K}_i^{\mathrm{f}} = \mathfrak{A}_i T^{\mathfrak{b}_i} \exp\big(-\mathfrak{E}_i/R_{\mathrm{g}}T\big), \qquad i \in \mathfrak{R},$$

where $\mathfrak{A}_i$ is the preexponential factor, $\mathfrak{b}_i$ the temperature exponent and $\mathfrak{E}_i$ the activation energy of the ith reaction.

2.3 Transport fluxes

The transport fluxes $\boldsymbol{\Pi}$, $\boldsymbol{\mathcal{F}}_k$, $k \in S$, and $\boldsymbol{Q}$ due to macroscopic variable gradients can be written in the form [7, 8, 9, 11, 12, 13]

$$\boldsymbol{\Pi} = -\kappa(\boldsymbol{\partial}_x\cdot\boldsymbol{v})\boldsymbol{I} - \eta\big(\boldsymbol{\partial}_x\boldsymbol{v} + \boldsymbol{\partial}_x\boldsymbol{v}^t - \tfrac{2}{3}(\boldsymbol{\partial}_x\cdot\boldsymbol{v})\boldsymbol{I}\big), \tag{2.4}$$

$$\boldsymbol{\mathcal{F}}_k = -\sum_{l\in S} C_{kl}\boldsymbol{d}_l - \rho Y_k \theta_k \boldsymbol{\partial}_x \log T, \qquad k \in S, \tag{2.5}$$

$$\boldsymbol{Q} = \sum_{k\in S} h_k \boldsymbol{\mathcal{F}}_k - \widehat{\lambda}\,\boldsymbol{\partial}_x T - p\sum_{k\in S} \theta_k \boldsymbol{d}_k, \tag{2.6}$$

with

$$\boldsymbol{d}_k = \frac{\boldsymbol{\partial}_x p_k}{p}, \quad k \in S,$$

where κ denotes the volume viscosity, η the shear viscosity, $\boldsymbol{I}$ the three dimensional identity tensor, C_{kl}, $k,l \in S$, the multicomponent flux diffusion coefficients, $\boldsymbol{d}_k$, $k \in S$, the species diffusion driving forces, θ_k, $k \in S$, the species thermal diffusion coefficients, $\widehat{\lambda}$ the partial thermal conductivity, and ^{t} the transposition operator. When the mass fractions are nonzero, it is also possible to define the species diffusion velocities $\boldsymbol{V}_k$, $k \in S$, by

$$\boldsymbol{V}_k = \frac{\boldsymbol{\mathcal{F}}_k}{\rho Y_k} = -\sum_{l \in S} D_{kl}\boldsymbol{d}_l - \theta_k \boldsymbol{\partial}_x \log T, \qquad k \in S,$$

where $D_{kl} = C_{kl}/\rho Y_k$, $k,l \in S$, are the multicomponent diffusion coefficients.

One may also introduce the alternative formulation [7, 11, 12, 13]

$$\boldsymbol{\mathcal{F}}_k = -\sum_{l \in S} C_{kl}(\boldsymbol{d}_l + X_l \widetilde{\chi}_l \boldsymbol{\partial}_x \log T), \qquad l \in S, \tag{2.7}$$

$$q = \sum_{k \in S} h_k \boldsymbol{\mathcal{F}}_k - \lambda \boldsymbol{\partial}_x T + R_{\mathrm{g}} T \sum_{k \in S} (\widetilde{\chi}_k / m_k) \boldsymbol{\mathcal{F}}_k. \tag{2.8}$$

where $\widetilde{\chi}_k$, $k \in S$, are the reduced thermal diffusion ratios and λ the thermal conductivity. The above expressions are more practical for mathematical purposes or for numerical simulations than the usual formulations (2.5) and (2.6).

The multicomponent transport coefficients κ, η, λ, $\widehat{\lambda}$, $C = (C_{kl})_{k,l \in S}$, $D = (D_{kl})_{k,l \in S}$, $\theta = (\theta_k)_{k \in S}$, or $\widetilde{\chi} = (\widetilde{\chi}_k)_{k \in S}$, are smooth functions of the state variables which are not explicitely given by the kinetic theory. These transport coefficients have important symmetry properties inherited from the underlying kinetic framework [7, 9, 13] and their evaluation requires solving linear systems as discussed in Section 7. The matrices C and D are generally irreducible and the governing equations have thus a complex structure [7]. The importance of the volume viscosity κ for compressible flows is further discussed in Section 7.

2.4 Mathematical assumptions

The species of the mixture are assumed to be constituted by atoms, and we denote by $\mathfrak{a}_{il}$ the number of lth atom in the ith species, $\mathfrak{A} = \{1, \dots, n^{\mathrm{a}}\}$ the set of atom indices, and $n^{\mathrm{a}} \geqslant 1$ the number of atoms—or elements—in the mixture. The assumptions on the coefficients are deduced form the kinetic theory of gases and are typically in the following form [7].

(H_1) *The molar masses m_k, $k \in S$, and the perfect gas constant R_{g} are positive constants. The formation energies e_k^{st}, $k \in S$, and entropies s_k^{st}, $k \in S$, are real constants. The specific heats c_{vk}, $k \in S$, are C^∞ functions of $T \in [0, \infty)$. There exist positive constants $\underline{c}_v$ and $\overline{c}_v$ such that $0 < \underline{c}_v \leqslant c_{vk}(T) \leqslant \overline{c}_v$ for $T \geq 0$ and $k \in S$.*

(H_2) *The stoichiometric coefficients ν_{ki}^{f} and ν_{ki}^{b}, $k \in S$, $i \in \mathfrak{R}$, the atomic coefficients $\mathfrak{a}_{kl}$, $k \in S$, $l \in \mathfrak{A}$, are nonnegative integers. The atom vectors $\mathfrak{a}_l$, $l \in \mathfrak{A}$, defined by $\mathfrak{a}_l = (\mathfrak{a}_{1l}, \dots, \mathfrak{a}_{nl})^t$, and the reaction vectors ν_i, $i \in \mathfrak{R}$, defined by $\nu_i = (\nu_{1i}, \dots, \nu_{ni})^t$, where $\nu_{ki} = \nu_{ki}^{\mathrm{b}} - \nu_{ki}^{\mathrm{f}}$, satisfy the mass conservation constraints $\langle \nu_i, \mathfrak{a}_l \rangle = 0$, $i \in \mathfrak{R}$, $l \in \mathfrak{A}$. The atom masses $\widetilde{m}_l$, $l \in \mathfrak{A}$, are positive constants, and the species molar masses m_k, $k \in S$, are given by $m_k = \sum_{l \in \mathfrak{A}} \widetilde{m}_l \, \mathfrak{a}_{kl}$.*

(H_3) *The reaction constants $\mathcal{K}_i^{\mathrm{f}}$, and $\mathcal{K}_i^{\mathrm{b}}$, $i \in \mathfrak{R}$, are C^∞ positive functions of $T > 0$ and satisfy the reciprocity relations $\mathcal{K}_i^{\mathrm{f}}(T) = \mathcal{K}_i^{\mathrm{b}}(T)\mathcal{K}_i^{\mathrm{e}}(T)$, $i \in \mathfrak{R}$.*

(H_4) *The flux diffusion matrix $C = (C_{kl})_{k,l \in S}$, the reduced thermal diffusion ratios vector $\widetilde{\chi} = (\widetilde{\chi}_1, \dots, \widetilde{\chi}_n)^t$, the volume viscosity κ, the shear viscosity η, and the thermal conductivity λ are C^∞ functions of $(T, \rho_1, \dots, \rho_n)$ for $T > 0$ and $\rho_i > 0$, $i \in S$. These coefficients also satisfy the mass conservation constraints $N(C) = \mathbb{R}Y$, $R(C) = \mathcal{U}^\perp$, $\widetilde{\chi} \in X^\perp$ where $Y = (Y_1, \dots, Y_n)^t$, $Y_k = \rho_k/\rho$, $\mathcal{U} = (1, \dots, 1)^t$ and $X = (X_1, \dots, X_n)^t$.*

(H_5) *The thermal conductivity λ and the shear viscosity η are positive. The volume viscosity κ is nonnegative. For $Y > 0$, the diffusion matrix $D = (1/\rho)\mathcal{Y}^{-1}C$ is symmetric positive semi-definite and its nullspace is $N(D) = \mathbb{R}Y$, where $\mathcal{Y} = \mathrm{diag}(Y_1, \dots, Y_n)$.*

Throughout these notes, for any matrix A, we denote by $N(A)$ its nullspace and $R(A)$ its range. The assumptions for transport coefficients when some mass fractions are vanishing are more complex [7] and are discussed in Section 4.

2.5 Entropy production

From Gibbs' relation $T\,\mathbb{D}\mathcal{S} = \mathbb{D}\mathcal{E} - \sum_{k\in S} g_k\,\mathbb{D}\rho_k$, where $\mathbb{D}$ denotes the total derivative, and the properties of transport coefficients and chemical production rate, one may derive the following balance equation for $\rho s = \mathcal{S}$ in $\mathbb{R}^d$ where $1 \leqslant d \leqslant 3$ [7, 84]

$$\begin{aligned}
&\partial_t(\rho s) + \boldsymbol{\partial}_x\boldsymbol{\cdot}(\rho \boldsymbol{v} s) + \boldsymbol{\partial}_x\boldsymbol{\cdot}\big(\frac{\boldsymbol{Q}}{T} - \sum_{k\in S}\frac{g_k}{T}\boldsymbol{\mathcal{F}}_k\big) = \frac{3d\kappa + 2\eta(3-d)}{3dT}(\boldsymbol{\partial}_x\boldsymbol{\cdot}\boldsymbol{v})^2 \\
&+ \frac{\eta}{2T}\big(\boldsymbol{\partial}_x\boldsymbol{v} + \boldsymbol{\partial}_x\boldsymbol{v}^t - \tfrac{2}{d}(\boldsymbol{\partial}_x\boldsymbol{\cdot}\boldsymbol{v})\,\boldsymbol{I}\big)\boldsymbol{:}\big(\boldsymbol{\partial}_x\boldsymbol{v} + \boldsymbol{\partial}_x\boldsymbol{v}^t - \tfrac{2}{d}(\boldsymbol{\partial}_x\boldsymbol{\cdot}\boldsymbol{v})\,\boldsymbol{I}\big) \\
&+ \frac{\lambda}{T^2}\boldsymbol{\partial}_x T\boldsymbol{\cdot}\boldsymbol{\partial}_x T + \frac{p}{T}\sum_{k,l\in S} D_{kl}\big(\boldsymbol{d}_k + X_k\widetilde{\chi}_k\boldsymbol{\partial}_x \log T\big)\boldsymbol{\cdot}\big(\boldsymbol{d}_l + X_l\widetilde{\chi}_l\boldsymbol{\partial}_x \log T\big) \\
&+ \sum_{i\in\mathfrak{R}} R_{\mathrm{g}}\mathcal{K}_i^{\mathrm{s}}\big(\langle\mu,\nu_i^{\mathrm{f}}\rangle - \langle\mu,\nu_i^{\mathrm{b}}\rangle\big)\,\big(\exp\langle\mu,\nu_i^{\mathrm{f}}\rangle - \exp\langle\mu,\nu_i^{\mathrm{b}}\rangle\big),
\end{aligned} \tag{2.9}$$

where $\nu_i^{\mathrm{f}} = (\nu_{1i}^{\mathrm{f}},\dots,\nu_{ni}^{\mathrm{f}})^t$, $\nu_i^{\mathrm{b}} = (\nu_{1i}^{\mathrm{b}},\dots,\nu_{ni}^{\mathrm{b}})^t$, $i\in\mathfrak{R}$, $\mu_k(T,\rho_k) = m_k g_k/R_{\mathrm{g}}T$, $k\in S$, $\mu = (\mu_1,\dots,\mu_n)^t$, and where the symmetric reaction constant $\mathcal{K}_i^{\mathrm{s}}$ is defined from $\log\mathcal{K}_i^{\mathrm{s}} = \log\mathcal{K}_i^{\mathrm{f}} - \langle M\nu_i^{\mathrm{f}},\mu^{\mathrm{u}}\rangle = \log\mathcal{K}_i^{\mathrm{b}} - \langle M\nu_i^{\mathrm{b}},\mu^{\mathrm{u}}\rangle$, with $\mu_k^{\mathrm{u}}(T) = \mu_k(T,m_k)$, $k\in S$. Entropy production therefore appears as a sum of nonnegative terms.

3 The Cauchy problem

The equations governing multicomponent reactive flows as derived from the kinetic theory of gases have local regular solutions [21] and global regular solutions around constant equilibrium states [20]. The method of proof relies on the symmetric normal form of the governing equations, on entropic estimates, and on the local dissipativity properties of the linearized equations. The smooth dependence on a parameter is also investigated in [24].

3.1 Vector notation

The equations governing multicomponent flows can be rewritten in the compact vector form

$$\partial_t U + \sum_{i\in C}\partial_i F_i + \sum_{i\in C}\partial_i F_i^{\mathrm{dis}} = \Omega, \tag{3.1}$$

where U is the conservative variable, ∂_i the spatial derivative operator in the ith direction, $C = \{1,\dots,d\}$ the indexing set of spatial directions, $d\in\{1,2,3\}$ the spatial dimension, F_i the convective flux in the ith direction, F_i^{dis} the dissipative flux in the ith direction, and Ω the source term. The conservative variable U is given by

$$U = \Big(\rho_1,\dots,\,\rho_n,\,\rho v_1,\dots,\,\rho v_d,\,\mathcal{E} + \tfrac{1}{2}\rho\boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{v}\Big)^t, \tag{3.2}$$

wheras the convective and diffusive fluxes F_i and F_i^{dis} in the ith direction can be written

$$\begin{aligned}
F_i &= \Big(\rho_1 v_i,\dots,\,\rho_n v_i,\,\rho v_1 v_i + \delta_{i1}p,\dots,\,\rho v_d v_i + \delta_{id}p,\,(\mathcal{E} + \tfrac{1}{2}\rho\boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{v} + p)v_i\Big)^t, \\
F_i^{\mathrm{dis}} &= \Big(\mathcal{F}_{1i},\dots,\,\mathcal{F}_{ni},\,\varPi_{i1},\dots,\,\varPi_{id},\,\mathcal{Q}_i + \sum_{j\in C}\varPi_{ij}v_j\Big)^t,
\end{aligned}$$

where δ_{ij} denotes the Kronecker symbol, v_i the velocity in the ith direction, $\mathcal{F}_{ki}$ the diffusion flux of the kth species in the ith direction, $\mathcal{Q}_i$ the heat flux in the ith direction, $\boldsymbol{\varPi} = (\varPi_{ij})_{i,j\in C}$ the viscous tensor so that $\boldsymbol{v} = (v_1,\dots,v_d)^t$, $\boldsymbol{\mathcal{F}}_k = (\mathcal{F}_{k1},\dots,\mathcal{F}_{kd})^t$, and $\boldsymbol{Q} = (\mathcal{Q}_1,\dots,\mathcal{Q}_d)^t$.

The map $Z \to U$ where $Z = (\rho_1,\dots\rho_n, v_1,\dots,v_d,T)^t$ is then a C^∞ diffeomorphism from the open set $(0,\infty)^n\times\mathbb{R}^d\times(0,\infty)$ onto a convex open set $\mathcal{O}_U$ of $\mathbb{R}^{\mathsf{n}}$ where $\mathsf{n} = n+d+1$. Denoting by $A_i = \partial_U F_i$, $i\in C$, the convective flux Jacobian matrices, B_{ij}, $i,j\in C$, the dissipation matrices defined in such a way that $\mathcal{F}_i = -\sum_{j\in C} B_{ij}(U)\partial_j U$ the dissipative flux in the ith direction, and Ω the source term, we obtain the qualinear system

$$\partial_t U + \sum_{i\in C} A_i(U)\partial_i U = \sum_{i,j\in C} \partial_i\Big(B_{ij}(U)\partial_j U\Big) + \Omega(U), \tag{3.3}$$

and all the system coefficients $A_i(U)$, $i \in C$, $B_{ij}(U)$, $i,j \in C$, and $\Omega(U)$, are smooth functions of U on the open convex set $\mathcal{O}_U$.

Note that we only investigate here the equations governing ideal mixture of perfect gases and we refer to [23, 25, 26, 29, 30] for other models and global existence with large data.

3.2 Entropy and symmetrization

Symmetrization properties of second order dissipative systems [14, 15, 16, 17, 18, 20, 21, 24, 27, 31] generalize classical results about hyperbolic systems [19, 22, 28] and can be applied to the equations governing multicomponent flows [20].

Proposition 3.1. *Consider the mathematical entropy $-\mathcal{S}$ and the corresponding entropic variable $V = -\big(\partial_U \mathcal{S}\big)^t$ given by*

$$V = (1/T)\big(g_1 - \tfrac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v}, \ldots, \, g_n - \tfrac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v}, \, v_1, \ldots, \, v_d, \, -1\big)^t. \tag{3.4}$$

Then $U \to V$ is a C^∞ diffeomorphism from the open set $\mathcal{O}_U$ onto the open set $\mathcal{O}_V = \mathbb{R}^{n+d} \times (-\infty, 0)$. Performing the change of variable $U = U(V)$, the system (3.3) is transformed into

$$\widetilde{A}_0(V)\partial_t V + \sum_{i\in C} \widetilde{A}_i(V)\partial_i V = \sum_{i,j\in C} \partial_i\Big(\widetilde{B}_{ij}(V)\partial_j V\Big) + \widetilde{\Omega}(V), \tag{3.5}$$

where $\widetilde{A}_0 = \partial_V U$, $\widetilde{A}_i = A_i\widetilde{A}_0$, $\widetilde{B}_{ij} = B_{ij}\widetilde{A}_0$, $\widetilde{\Omega} = \Omega$, and $\widetilde{A}_0(V)$ is symmetric positive definite, $\widetilde{A}_i(V)$, $i \in C$, are symmetric, we have the reciprocity relations $\widetilde{B}_{ij}(V)^t = \widetilde{B}_{ji}(V)$, $i,j \in C$, and $\widetilde{B}(V,w) = \sum_{i,j\in C} \widetilde{B}_{ij}(V)w_i w_j$ is symmetric positive semi-definite for w in the sphere Σ^{d-1} and $V \in \mathcal{O}_V$.

The symmetrizability properties of second order systems of partial differential equations are closely associated with the notion of entropy and we refer to [15, 18, 20] for more details. It is important to note that such a symmetric structure is the consequence of the underlying kinetic framework, that is, of symmetry properties deduced from that of the Boltzmann collision operator [7].

3.3 Normal forms

The symmetric system (3.5) may be rewritten into a normal form, that is, in the form of a symmetric hyperbolic-parabolic composite system, where hyperbolic and parabolic variables are split [14, 15, 16, 17, 18, 20, 21, 27, 31]. We use in particular a characterization of all possible normal forms for symmetrizable systems of partial differential equations such that the nullspace of $\widetilde{B}(V,w)$ is invariant [20]. This characterization of normal variables, written here in the special situation of multicomponent reactive flows, holds for general systems of conservation laws [20]. The parameter dependent case has also been investigated [24].

Theorem 3.2. *Consider a diffeomorphism $V \longmapsto W$ from $\mathcal{O}_V$ onto an open set $\mathcal{O}_W$. Performing the change of variable $V = V(W)$, and multiplying of the left by the transpose of the Jacobian matrix $\partial_W V^t$, the system (3.5) is transformed into*

$$\begin{aligned}\overline{A}_0(W)\partial_t W &+ \sum_{i\in C} \overline{A}_i(W)\partial_i W \\ &= \sum_{i,j\in C} \partial_i\Big(\overline{B}_{ij}(W)\partial_j W\Big) + \overline{\mathcal{T}}(W, \partial_x W) + \overline{\Omega}(W),\end{aligned} \tag{3.6}$$

where

$$\overline{A}_0 = \partial_W V^t \widetilde{A}_0 \partial_W V, \qquad \overline{B}_{ij} = \partial_W V^t \widetilde{B}_{ij} \partial_W V,$$

$$\overline{A}_i = \partial_W V^t \widetilde{A}_i \partial_W V, \quad \overline{\mathcal{T}} = -\sum_{i,j\in C} \partial_i(\partial_W V^t)(\widetilde{B}_{ij}\partial_W V)\partial_j W, \quad \overline{\Omega} = \partial_W V^t \widetilde{\Omega}.$$

The system (3.6) *is said to be in the normal form and W is said to be a normal variable when $\{1,\dots,\mathsf{n}\}$ may be partitioned into the sets $\mathrm{I} = \{1,\dots,\mathsf{n}_0\}$ and $\mathrm{II} = \{\mathsf{n}_0+1,\dots,n+d+1\}$, such that*

$$\overline{A}_0 = \begin{pmatrix} \overline{A}_0^{\mathrm{I},\mathrm{I}} & 0 \\ 0 & \overline{A}_0^{\mathrm{II},\mathrm{II}} \end{pmatrix}, \qquad \overline{B}_{ij} = \begin{pmatrix} 0 & 0 \\ 0 & \overline{B}_{ij}^{\mathrm{II},\mathrm{II}} \end{pmatrix},$$

the matrix $\overline{B}^{\mathrm{II},\mathrm{II}}(W,w) = \sum_{i,j\in C} \overline{B}_{ij}^{\mathrm{II},\mathrm{II}}(W) w_i w_j$ is positive definite for $W \in \mathcal{O}_W$ and $w \in \Sigma^{d-1}$, and we have $\overline{\mathcal{T}}(W,\partial_x W) = \big(\overline{\mathcal{T}}_{\mathrm{I}}(W,\partial_x W_{\mathrm{II}}), \overline{\mathcal{T}}_{\mathrm{II}}(W,\partial_x W)\big)^t$.

Then all normal forms of the system (3.5) *are obtained with variables W in the form*

$$W = \Big(W_{\mathrm{I}}(\rho), W_{\mathrm{II}}\Big(\frac{g_2-g_1}{T}, \dots, \frac{g_n-g_1}{T}, \frac{v_1}{T}, \dots, \frac{v_d}{T}, \frac{-1}{T} \Big)\Big)^t, \tag{3.7}$$

where I corresponds to the hyperbolic component and II to the parabolic components. Moreover we have $\overline{\mathcal{T}}(W,\partial_x W) = \big(0, \overline{\mathcal{T}}_{\mathrm{II}}(W,\partial_x W_{\mathrm{II}})\big)^t$, and if W_{II} depends linearly on $\big(g_2-g_1,\dots,\, g_n-g_1,\, v_1,\dots,\, v_d,\, -1\big)/T$ then $\overline{\mathcal{T}}(W,\partial_x W) = 0$.

Corollary 3.3. *Consider the diffeomorphism $V \longmapsto W$ from $\mathcal{O}_V$ onto the open set $\mathcal{O}_W = (0,\infty) \times \mathbb{R}^{n-1} \times \mathbb{R}^d \times (0,\infty)$ given by*

$$W = \big(\rho,\, \log(\rho_2^{r_2}/\rho_1^{r_1}), \dots, \log(\rho_n^{r_n}/\rho_1^{r_1}),\, v_1, \dots, v_d,\, T\big)^t, \tag{3.8}$$

where $r_k = R_{\mathrm{g}}/m_k$. Then W is a normal variable and the equations (3.6) *are in normal form.*

Various normal forms are computed explicitly in [20] in particular for the above variable (3.8) and also for the 'natural' normal variable

$$W = \Big(\rho, \frac{g_2-g_1}{T}, \dots, \frac{g_n-g_1}{T}, \frac{v_1}{T}, \dots, \frac{v_d}{T}, \frac{-1}{T}\Big)^t, \tag{3.9}$$

which is useful in the context of chemical equilibrium flows.

3.4 Local dissipativity

We present in this section the dissipativity properties around equilibrium states that are needed in order to establish global existence and asymptotic stability [15, 20]. The existence of equilibrium points is a consequence of the structural properties of thermochemistry [7].

Proposition 3.4. *For $T^{\mathrm{e}} > 0$ and $(\rho_1^{\mathrm{c}},\dots,\rho_n^{\mathrm{c}})^t \in (0,\infty)^n$, there exists a unique equilibrium point U^{e} associated with $Z^{\mathrm{e}} = \big(\rho_1^{\mathrm{e}},\dots,\rho_n^{\mathrm{e}}, v_1^{\mathrm{e}},\dots,v_d^{\mathrm{e}}, T^{\mathrm{e}}\big)^t$ such that $v_i^{\mathrm{e}} = 0$, $i \in C$, and $(\rho_1^{\mathrm{e}} - \rho_1^{\mathrm{c}},\dots,\rho_n^{\mathrm{e}} - \rho_n^{\mathrm{c}})^t \in$ Span$\{\, M\nu_i,\ i \in \mathfrak{R}\,\}$ where $M = \mathrm{diag}(m_1,\dots,m_n)$.*

The system of partial differential equations governing multicomponent reactive flows written in normal form is also strictly dissipative and the source terms are locally stable [15, 16, 18, 20, 24].

Proposition 3.5. *The matrix $\overline{A}_0(W^{\mathrm{e}})$ is symmetric positive definite, the matrices $\overline{A}_i(W^{\mathrm{e}})$, $i \in C$, are symmetric, we have $\overline{B}_{ij}(W^{\mathrm{e}})^t = \overline{B}_{ji}(W^{\mathrm{e}})$, $i,j \in C$, and the linearized source terms $\overline{L}(W^{\mathrm{e}}) = -\partial_W \overline{\Omega}(W^{\mathrm{e}})$ are symmetric positive semi-definite. Moreover, the linearized normal form is strictly dissipative in the sense that the eigenvalues $\lambda(\zeta,w)$ of the problem*

$$\lambda \overline{A}_0(W^{\mathrm{e}})\phi + \Big(\zeta \sum_{i\in C} \overline{A}_i(W^{\mathrm{e}}) w_i - \zeta^2 \sum_{i,j\in C} \overline{B}_{ij}(W^{\mathrm{e}}) w_i w_j + \overline{L}(W^{\mathrm{e}})\Big)\phi = 0,$$

for $\zeta \in \mathrm{i}\,\mathbb{R}\backslash\{0\}$ and $w \in \Sigma^{d-1}$, have a negative real part.

Proposition 3.6. *The smallest linear space containing the source term $\widetilde{\Omega}(V) = \Omega\big(U(V)\big)$ for any $V \in \mathcal{O}_V$ in included in the range $\widetilde{L}(V^{\mathrm{e}}) = -(\partial_V \widetilde{\Omega})(V^{\mathrm{e}})$. Moreover, there exists a neighborhood of V^{e} in $\mathcal{O}_V$ and a positive constant α such that for any V in this neighborhood we have*

$$\alpha\,\big|\,\widetilde{\Omega}(V)\big|^2 \leqslant -\big\langle V - V^{\mathrm{e}},\, \widetilde{\Omega}(V)\big\rangle.$$

3.5 Existence of solutions

The local dissipativity properties now imply global existence and asymptotic stability of equilibrium states [15, 20, 24].

Theorem 3.7. *Let $d \geqslant 1$, $l \geqslant [d/2]+2$ and $W^0(x)$ such that $\|W^0 - W^{\mathrm{e}}\|_{H^l}$ is small enough. The Cauchy problem with initial conditions $W(0,x) = W^0(x)$ has a global solution such that*

$$W_{I} - W_{I}^{\mathrm{e}} \in C^0\big([0,\infty); H^l\big) \cap C^1\big([0,\infty); H^{l-1}\big), \tag{3.10}$$

$$W_{II} - W_{II}^{\mathrm{e}} \in C^0\big([0,\infty); H^l\big) \cap C^1\big([0,\infty); H^{l-2}\big). \tag{3.11}$$

Moreover we have the estimates

$$\|W(t) - W^{\mathrm{e}}\|_{H^l}^2 + \int_0^t \big(\|\partial_x W_{I}(\tau)\|_{H^{l-1}}^2 + \|\partial_x W_{II}(\tau)\|_{H^l}^2\big)\, d\tau \leqslant C\|W^0 - W^{\mathrm{e}}\|_{H^l}^2,$$

and $\sup_{\mathbb{R}^d} |W(t) - W^{\mathrm{e}}|$ *goes to zero as $t \to \infty$.*

Theorem 3.8. *Let $d \geqslant 1$, $l \geqslant [d/2]+3$ and assume that the initial condition $W^0(x)$ is such that $W^0 - W^{\mathrm{e}} \in H^l(\mathbb{R}^d) \cap L^p(\mathbb{R}^d)$, where $p = 1$, if $d = 1$, and $p \in [1,2)$, if $d \geqslant 2$. Then if $\|W^0 - W^{\mathrm{e}}\|_{H^l} + \|W^0 - W^{\mathrm{e}}\|_{L^p}$ is small enough, the global solution satisfy the dacay estimate*

$$\|W(t) - W^{\mathrm{e}}\|_{H^{l-2}} \leqslant \beta(1+t)^{-\gamma}\big(\|W^0 - W^{\mathrm{e}}\|_{H^{l-2}} + \|W^0 - W^{\mathrm{e}}\|_{L^p}\big),$$

for $t \in [0,\infty)$, where β is a positive constant and $\gamma = d \times (1/2p - 1/4)$.

4 Anchored waves

Traveling waves in inert or reactive flows can be classified into deflagration and detonation waves [32]. In the context of combustion—which does not decrease the problem generality but makes things more explicit—weak deflagrations correspond to plane laminar flames. The anchored flame problem has been investigated with complex chemistry and detailed transport by using entropic estimates and the Leray-Schauder topological degree theory[36].

A difficulty typically associated with waves in reactive media extending over $(-\infty, +\infty)$ is that limit points have to be equilibrium points where source terms vanish. However, chemical source terms generally only have a unique equilibrium point in a given atom conservation manifold [7]. In the context of combustion this is the cold boundary difficulty. For unsteady flows, the solution is to use unsteady boundary conditions as suggested by Zeldovitch and investigated mathematically by Roquejoffre [33]. For steady waves, on the other hand, the proper physical model is the anchored wave model [36].

4.1 Plane flame equations

The equations governing plane flames can be derived from the general equations presented in Section 2 upon using the low Mach number limit, stationarity, and the one-dimensional geometry. Denoting by x the coordinate normal to the flame, the conservation of species mass and energy are found in the form

$$c\, Y_k' + \mathcal{F}_k' = m_k \omega_k, \quad k \in S, \tag{4.1}$$

$$c\, h' + q' = 0, \tag{4.2}$$

where c denotes the mass flow rate, $'$ the spatial derivation with respect to x, $\boldsymbol{\mathcal{F}}_k = (\mathcal{F}_k, 0, 0)^t$ the mass flux of the kth species, $h = \mathcal{H}/\rho$ the enthalpy per unit mass, and $\boldsymbol{Q} = (q, 0, 0)^t$ the heat flux. The unknowns are the mass flow rate c—which is a nonlinear eigenvalue—the mass fractions $Y = (Y_1, \ldots, Y_n)^t$ and the enthalpy h, or equivalently the temperature T. The momentum equation uncouples and may only be used to evaluate a pressure corrector [32, 36, 7].

The mass fractions naturally appear in the governing equations (4.1) so that it is more convenient to use these variables rather than the species partial densities. The enthalpy h is for instance written in the form $h = \sum_{k\in S} Y_k h_k(T)$ where $h_k(T) = h_k^{\mathrm{st}} + \int_{T^{\mathrm{st}}}^{T} c_{pk}(t)\, dt$ where h_k^{st} denotes the formation enthalpy of the kth species at temperature T^{st}, $c_{pk} = c_{vk} + R_{\mathrm{g}}/m_k$ the specific heat of the kth species at constant pressure, and the specific entropy $s = \mathcal{S}/\rho$ is rewritten in a similar way [36]. It is also more convenient and more elegant to consider all the mass fractions as independent unknowns and to recover the relation $\sum_{k\in S} Y_k = 1$ from the species equations and boundary conditions.

In the small Mach number limit, the transport fluxes $\mathcal{F}_k$, $k \in S$, and q are simplified in the form

$$\mathcal{F}_k = -\sum_{l\in S} C_{kl}(X_l' + X_l \widetilde{\chi}_l T'/T), \qquad k \in S, \tag{4.3}$$

$$q = \sum_{k\in S} (h_k + R_{\mathrm{g}} T \widetilde{\chi}_k/m_k)\mathcal{F}_k - \lambda T'. \tag{4.4}$$

All the species second derivatives are thus coupled through the flux matrix C and are coupled with the temperature second derivative through the thermal diffusion coefficients $\widetilde{\chi}$.

Remark 4.1. *The following temperature equation is obtained from* (4.1)–(4.4)

$$c\, c_p T' = \Big(\lambda T' - R_{\mathrm{g}} T \sum_{l\in S} (\widetilde{\chi}_l/m_l)\mathcal{F}_l\Big)' - \sum_{k\in S} c_{pk} T' \mathcal{F}_k - \sum_{k\in S} h_k m_k \omega_k,$$

where $c_p = \sum_{k\in S} Y_k c_{pk}$. This equation notably contain quadratic derivative terms $\sum_{k\in S} c_{pk} T' \mathcal{F}_k$ and a priori unbounded source terms $\sum_{k\in S} h_k m_k \omega_k$. The presence of thermal diffusion terms $\sum_{l\in S} (\widetilde{\chi}_l/m_l)\mathcal{F}_l$ also prohibits the use of the maximum principle.

4.2 Boundary conditions for anchored flames

The boundary conditions at the origin are that of the anchored flame model

$$c(Y_k(0) - Y_k^{\mathrm{f}}) + \mathcal{F}_k(0) = 0, \quad k \in S, \qquad c(h(0) - h^{\mathrm{f}}) + q(0) = 0, \qquad T(0) = T^{\mathrm{i}},$$

where $(T^{\mathrm{f}}, Y^{\mathrm{f}})$ is a state out of equilibrium and T^{i} a temperature such that $T^{\mathrm{f}} < T^{\mathrm{i}}$. This model has first been introduced by Hirschfelder, Curtiss and Campbell [34] and represents an adiabatic porous burner located at the origin. The boundary conditions in the hot gases are

$$Y_k(\infty) = Y_k^{\mathrm{e}}, \quad k \in S, \qquad T(\infty) = T^{\mathrm{e}},$$

where $(T^{\mathrm{e}}, Y^{\mathrm{e}})$ is an equilibrium state whose existence and uniqueness can be deduced form the structure of thermochemistry under natural assumptions on $(T^{\mathrm{f}}, Y^{\mathrm{f}})$ and it is also assumed that $T^{\mathrm{i}} < T^{\mathrm{e}}$ [35, 36]. We then look for smooth solutions (T, Y, c) of the anchored flame model such that $T > 0$, $Y \geqslant 0$, $Y \neq 0$, and $c > 0$.

One may also replace the boundary conditions at the origin by $T(-\infty) = T^{\mathrm{f}}$, $Y(-\infty) = Y^{\mathrm{f}}$ and $T(0) = T^{\mathrm{i}}$. In this situation, it is necessary to replace the source term ω by $H\omega$ where H is the Heavyside function. One may establish that this formulation over $(-\infty, \infty)$ is equivalent to that of the anchored flame over $[0, \infty)$. Any solution of the anchored flame model may be extended over $(-\infty, 0)$ and satisfies $T(-\infty) = T^{\mathrm{f}}$ and $Y(-\infty) = Y^{\mathrm{f}}$.

4.3 Further mathematical assumptions

Since we are now interested in solutions which are not in the neighborhood of an equilibrium solution, it is necessary to specify the behavior of transport coefficients for vanishing mass fractions as well as for large or small temperatures. The following assumptions have been derived from the properties of transport linear systems [7, 13, 35, 36].

($\mathsf{H_6}$) *For $Y \geqslant 0$, $Y \neq 0$, we define the sets $S^+ = \{\, k \in S,\ Y_k > 0 \,\}$ and $S^0 = \{\, k \in S,\ Y_k = 0 \,\}$, and we denote by Υ the permutation matrix associated with the reordering of S into (S^+, S^0). We then have the block structure*

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

where C^{00} is a diagonal matrix with positive diagonal coefficients and where D^{++} defined by $\rho D^{++}_{kl} = C^{++}_{kl}/Y_k$, $k,l \in S^+$, is symmetric positive semi-definite with nullspace $\mathbb{R}Y^+$ where Y^+ corresponds to the S^+ mixture, that is, $Y = \Upsilon(Y^+, 0)^t$.

($\mathsf{H_7}$) *There exists a positive function $\varphi(T)$ defined for $T > 0$ such that the reduced coefficients $C^0(T,Y) = C(T,Y)/\varphi(T)$, $\lambda^0(T,Y) = \lambda(T,Y)/\varphi(T)$, and $\widetilde{\chi}^0(T,Y) = \widetilde{\chi}(T,Y)$ have continuous extensions for $T \in [0,\infty]$, $Y \geqslant 0$, $Y \neq 0$, which satisfy* (H_4)–(H_5).

The function φ depends on the interaction potentials between pairs of particles [35, 36] and for rigid spheres we have for instance $\varphi(T) = \sqrt{T}$ [11, 12]. One of the main difficulties associated with the model, which takes into account multicomponent transport, is to correlate the fluxes and the gradients. This can only be done by using the entropy s thanks to the properties of the source terms and of the transport coefficients [36].

Lemma 4.2. *Denoting by s the specific entropy and $\psi = (q - \sum_{k\in S} g_k \mathcal{F}_k)/T$ the entropy flux, we have*

$$c\, s' + \psi' = \mathfrak{v} = \lambda(T'/T)^2 + \frac{p}{T}\sum_{k,l\in S} D_{kl}\big(X_k' + X_k\widetilde{\chi}_k T'/T\big)\,\big(X_l' + X_l\widetilde{\chi}_l T'/T\big)$$

$$+ \sum_{i\in\mathfrak{R}} R_{\mathrm{g}}\mathcal{K}_i^{\mathrm{s}}\Big(\langle\mu,\nu_i^{\mathrm{f}}\rangle - \langle\mu,\nu_i^{\mathrm{b}}\rangle\Big)\,\Big(\exp\langle\mu,\nu_i^{\mathrm{f}}\rangle - \exp\langle\mu,\nu_i^{\mathrm{b}}\rangle\Big), \qquad (4.5)$$

where we use notation similar to that of Section 2.5.

In order to use (4.5) we must control λ and the quadratic form associated with D on the physical hyperplane $\mathcal{U}^\perp$ where $\mathcal{U} = (1,\dots,1)^t$. A comprehensive investigation of multicomponent transport [35, 36] establishes that there exists a constant $\delta > 0$ such that $\delta\varphi \leqslant \lambda \leqslant (1/\delta)\varphi$ and

$$\forall x \in \mathcal{U}^\perp \subset \mathbb{R}^n, \qquad \delta\varphi\sum_{k\in S}\frac{x_k^2}{Y_k} \leqslant \frac{p}{T}\sum_{k,l\in S} D_{kl}x_kx_l \leqslant (1/\delta)\varphi\sum_{k\in S}\frac{x_k^2}{Y_k}.$$

This inequality reveals that the natural norm of multicoponent diffusion is not the usual Sobolev norm but involve the mass fractions at the denominator of the mass fraction gradients squared [35, 36].

4.4 Existence on a bounded domain

In order to establish the existence of solutions, we first consider the anchored flame problem on a bounded domain $[0,a]$ we use a fixed point formulation. The boundary conditions at a are written in the form $T(a) = T^{\mathrm{e}}$, $Y(a) = Y^{\mathrm{e}}$ and we use the Leray-Schauder topological degree theory. The main difficulty is to establish a priori estimates in order to show that the degree is well defined and to evaluate this degree with suitable homotopy pathes [36].

In order to simplify the presentation, we only state a few estimates for the flame equations over $[0,a]$. A first step is to establish that the species remain positive in order to be able to use the entropy estimates (4.5).

Lemma 4.3. *Let (T,Y,c) be a solution of the anchored flame problem over $[0,a]$ and let extend this solution over $(-\infty,0)$. Then one has $Y > 0$, $\sum_{k\in S} Y_k = 1$, $Y(-\infty) = Y^{\mathrm{f}}$, $T(-\infty) = T^{\mathrm{f}}$ and*

$$\int_{-\infty}^{a} \mathfrak{v}\, dx = c(s^{\mathrm{e}} - s^{\mathrm{f}}).$$

This entropic estimates allows to control the integrals of $\varphi\sum_{k\in S} Y_k'^2/Y_k$ and $\varphi(T'/T)^2$. The *fundamental* step is then the following L^∞ estimate on temperature [36].

Lemma 4.4. *Let (T,Y,c) be a solution of the anchored flame problem over the domain $[0,a]$. There exists positive constants α and β independent of a such that $\alpha < T < \beta$.*

A priori estimates fo the eigenvalue c require similar techniques and it is next possible to estimate the derivatives of T and Y at any order and to establish an existence theorem over $[0,a]$ using the homotopy invariance of the degree [36].

4.5 Existence of solutions

In order to let $a \to \infty$ it is important to derive estimates of the eigenvalue c independent of a. A fundamental tool is the exponential decrease of entropy dissipation rate residuals $\int_x^a \mathfrak{v}\, dx$ when (T, Y) remains close to the equilibrum state $(T^{\rm e}, Y^{\rm e})$ [35, 36]. This exponential decrease is obtained by using the entropy balance equation as well as a stability inequality due to Boillat and Pousin in the form

$$h(T,Y) = h^{\rm e}, \quad Y - Y^{\rm e} \in M\mathcal{R} \implies \delta\left(s^{\rm e} - s(T,Y)\right) \leqslant -\sum_{k\in S} \frac{g_k m_k \omega_k}{T},$$

where $\mathcal{R} = \mathrm{Vect}\{\nu_i,\ i \in \mathfrak{R}\}$. Such stability inequalities are established locally around equilibrium states and then globally when the chemical reaction mechanism does not have spurious 'boundary equilibrium points' in the atom conservation manifolds associated with $(T^{\rm e}, Y^{\rm e})$ [35, 36]. These exponential decrease rates next allow to prove the asymptotic behavior of the solution at infinity.

Theorem 4.5. *There exist constants $\bar{a}$, d and $\mathfrak{C}$ independent of a such that*

$$\forall a \geqslant \bar{a} \qquad \forall x \in [0,a], \qquad |T(x) - T^{\rm e}| + \|Y(x) - Y^{\rm e}\| \;\leqslant\; \mathfrak{C} \exp(-dx),$$

Finally, passing to the limit $a \to \infty$ and using a priori estimates independent of a one may establish the following result [7, 35, 36].

Theorem 4.6. *There exists a C^∞ solution to the anchored flame problem.*

5 Related models

In this section, we address fluid models whose mathematical structure is similar to that investigated in Section 3. We first discuss the Saint-Venant model and then chemical equilibrium flows. Other models are notably full vibrational nonequilibrium flows [21] as well as ambipolar plasmas [24].

5.1 Saint-Venant Equations

The Saint-Venant system of partial differential equations models shallow water flows as well as thin viscous sheets over fluid substrates like oil slicks, atlantic waters in the Strait of Gilbraltar or float glasses. Numerous existence results can be found in the literature concerning this system, which does not include an energy equation, in various functional settings. We refer the reader notably to Serre [19] and Dafermos [22] for inviscid models and to Lions [41] and Wang and Xu [42] for viscous Saint-Venant models with constant viscosity coefficients. Global weak solutions have also been investigated by Bresch [37], Bresch and Desjardins [38], Bresch, Desjardins, and Métivier [39], and Li, Li, and Xin [40] for the situation density dependent viscosities, using a gradient entropy [37], and Li, Li, and Xin [40] also considered the vanishing of vacuum states.

On the other hand, the Saint-Venant model with an energy equation and with temperature dependent transport coefficients has recently been investigated [43]. Modeling temperature variations is important in various environmental and engineering applications like float glasses. The full derivation of the model from the three dimensional incompressible Navier-Stokes equations has been conducted and the resulting system of partial differential equations shares a similar stucture with that investigated in Section 3. The correponding conservative variable is in the form

$$U = \left(\mathsf{h},\ \mathsf{h}u,\ \mathsf{h}v,\ \mathcal{E} + \tfrac{1}{2}\mathsf{h}(u^2+v^2)\right)^t, \tag{5.1}$$

where h is the vertical height of the viscous sheet or of the shallow water flow playing the rôle of a density, u, v are the horizontal components of the mass averaged flow velocity. The internal energy per unit volume of the fluid sheet is given by $\mathcal{E} = \mathsf{h}e$ where the internal energy per unit mass e can be written

$$e = e^{\rm st} + \int_{T^{\rm st}}^{T} c_v(\tau)\, d\tau + \tfrac{1}{2}\alpha\mathsf{h}, \tag{5.2}$$

where c_v is the heat capacity at constant volume per unit mass of the fluid, T the absolute temperature, $e^{\rm st}$ the formation energy of the fluid at the standard temperature $T^{\rm st}$, and α a parameter associated with gravity [43]. Note that, unlike for ideal gas mixtures, the specific internal energy e depends on the 'density' h.

The Saint-Venant quasilinear system of partial differential equations with a temperature equation admits an entropy and may be symmetrized. The resulting system is then shown to satisfy the nullspace invariance property and is recast into a normal form. The symmetrizing variable is notably obtained from the entropy and not the kinetic energy as is traditional in the isothermal case. Upon establishing the local dissipative structure of the linearized normal form, global existence results and asymptotic stability of equilibrium states are obtained [43].

5.2 Equilibrium flows

Chemical equilibrium flows are a limiting model which is of interest for various applications, such as chemical vapor deposition reactors [46], flows around space vehicles [1, 47], or diverging nozzle rocket flows [32]. These simplified models provide reasonable predictions when the characteristic chemical times are small in comparison with the flow time, and the associated computational costs are significantly reduced in comparison with chemical nonequilibrium models.

The equations governing chemical equilibrium flows may be derived by using two different methods. A first possibility is to take into account chemical equilibrium directly at the molecular level, that is, at the Boltzmann level. This model is the kinetic equilibrium regime introduced in [44] and further investigated in [45]. In this regime, by using an Enskog expansion, the corresponding macroscopic equations at chemical equilibrium are obtained. A second possibility is to start directly from the macroscopic equations at chemical nonequilibrium presented in Section 2 and to superimpose chemical equilibrium. It turns out, however, that both methods lead to the same conservations equations, transport fluxes, thermodynamics, as well as qualitative properties of transport coefficients [45]. Still note that these two methods yield different quantitative values for the transport coefficients [45]. We summarize the second method in the following.

When chemical equilibrium is superimposed in the conservation equations investigated in Section 2, it is then necessary to project the nonequilibrium equations onto the zero source term linear space and to write the algebraic chemical equilibrium constraint. *These chemical constraint are then used to eliminate the reactive part of the conservative variable and to reduce the equilibrium flow equations to a set of partial differential equations* [7]. The species and thermal variables needed to describe chemical equilibrium flows are found to be the atomic mass densities $\widetilde{\rho}_l = \sum_{k\in S} \widetilde{m}_l \mathfrak{a}_{kl} \rho_k / m_k$, $l \in \mathfrak{A}$, and the total energy per unit volume, which have to be completed by the momentum in each spatial direction. The corresponding conservative variable for chemical equilibrium flows is thus in the form

$$U = \Big(\widetilde{\rho}_1, \dots, \widetilde{\rho}_{n^{\mathfrak{a}}}, \, \rho v_1, \dots, \rho v_d, \, \mathcal{E} + \tfrac{1}{2} \rho \boldsymbol{v} \cdot \boldsymbol{v} \Big)^t .$$

The resulting system of partial differential equations is then symmetrizable and can be investigated as for nonequilibrium multicomponent reactive flows [7]. Upon establishing the local dissipative structure of the linearized normal form, global existence results and asymptotic stability of equilibrium states are obtained [7]. These results have recently been extended to the more general situation of partial equilibrium flows [48].

6 Magnetized flows

We investigate a system of partial differential equations modeling ionized magnetized reactive dissipative gas mixtures. In these models, the transport fluxes are anisotropic linear combinations of gradients and also include zeroth order contributions due to electromagnetic forces. There are also source terms depending on the solution gradients. A new definition of entropy is introduced and only partial symmetrization may be achieved as well as a partially normal form. Using a result of Vol'Pert and Hudjaev, we prove local existence and uniqueness of a bounded smooth solution to the Cauchy problem [51].

6.1 Governing equations

We consider the equations governing reactive ionized magnetized dissipative gas mixtures. These equations are derived from the kinetic theory of weakly ionized polyatomic reactive gas mixtures and can be split between conservation equations, transport fluxes, thermochemistry, and Maxwell's equations [49]. The resulting conservation equations are in the compact form

$$\partial_t U + \sum_{i\in C} \partial_i F_i + \sum_{i\in C} \partial_i F_i^{\mathrm{diss}} = \Omega^{\boldsymbol{j}}, \tag{6.1}$$

where ∂_t is the time derivative operator, ∂_i the space derivative operator in the ith direction, $C = \{1, 2, 3\}$ the indexing set of spatial coordinates, U the conservative variable, $\Omega^{\boldsymbol{j}}$ the full source term, F_i the convective flux in the ith direction, and F_i^{diss} the dissipative flux in the ith direction. The conservative variable U is given by

$$U = \Big(\rho_1, \dots, \rho_n, \rho\boldsymbol{v}, \boldsymbol{E}, \boldsymbol{B}, \mathcal{E} + \tfrac{1}{2}\rho\boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{v} + \varepsilon_0\boldsymbol{E}\boldsymbol{\cdot}\boldsymbol{E} + \tfrac{1}{\mu_0}\boldsymbol{B}\boldsymbol{\cdot}\boldsymbol{B}\Big)^t, \tag{6.2}$$

where ρ_k, $k \in S$, are the species partial mass densities, $S = \{1, \dots, n\}$ the species indexing set, n the number of species, $\rho = \sum_{k\in S} \rho_k$ the total mass density, $\boldsymbol{v}$ the mass average fluid velocity, $\boldsymbol{E}$ the electric field, $\boldsymbol{B}$ the magnetic field, ε_0 the dielectric constant in vacuum, μ_0 the magnetic permeability in vacuum, and $\mathcal{E}$ the internal energy per unit volume. For notational convenience, the three components of the velocity vector $\boldsymbol{v}$, the electric field $\boldsymbol{E}$, and the magnetic field $\boldsymbol{B}$, are written as three dimensional vectors in U and this notational shortcut is used throughout this Section. The source term $\Omega^{\boldsymbol{j}}$ reads

$$\Omega^{\boldsymbol{j}} = \big(m_1\omega_1, \dots, m_n\omega_n, \rho\boldsymbol{g} + q(\boldsymbol{E} + \boldsymbol{v}\wedge\boldsymbol{B}) + \boldsymbol{j}\wedge\boldsymbol{B}, -(q\boldsymbol{v} + \boldsymbol{j})/\varepsilon_0, \boldsymbol{0}, \rho\boldsymbol{g}\boldsymbol{\cdot}\boldsymbol{v}\big)^t, \tag{6.3}$$

where $m_k\omega_k$, $k \in S$, denote the species chemical production rates, $\boldsymbol{g}$ the gravity vector, $\boldsymbol{0}$ the three dimensional zero vector, $q = \sum_{k\in S} q_k$ the total charge per unit volume, q_k, $k \in S$, the species charge per unit volume, and the vector $\boldsymbol{j}$ denotes the conduction current $\boldsymbol{j} = \sum_{k\in S} q_k \boldsymbol{V}_k$.

The convective fluxes F_i, $i \in C$, are in the form

$$F_i = \big(v_i\rho_1, \dots, v_i\rho_n, \rho v_i\boldsymbol{v} + p\boldsymbol{e}^i, -\boldsymbol{e}^i\wedge\boldsymbol{B}/(\varepsilon_0\mu_0), \boldsymbol{e}^i\wedge\boldsymbol{E}, (\rho e^{\mathrm{t}} + p)v_i + P_i\big)^t, \tag{6.4}$$

where $\boldsymbol{e}^i$, $i \in C$, is the i^{e} canonical base vector of$\mathbb{R}^3$, p the thermodynamic pressure, and $\boldsymbol{P} = \boldsymbol{E}\wedge\boldsymbol{B}/\mu_0$ the Poynting vector. The diffusive fluxes F_i^{diss}, $i \in C$, are in the form

$$F_i^{\mathrm{diss}} = \big(\rho_1 V_{1i}, \dots, \rho_n V_{ni}, \mathit{\Pi}_{i\bullet}, \boldsymbol{0}, \boldsymbol{0}, \mathcal{Q}_i + \sum_{j\in C} \mathit{\Pi}_{ij} v_j\big)^t, \tag{6.5}$$

where $\boldsymbol{V}_k$, $k \in S$, are the species diffusion velocities, $\mathit{\Pi}_{i\bullet} = (\mathit{\Pi}_{1i}, \mathit{\Pi}_{2i}, \mathit{\Pi}_{3i})^t$ the ith column of the viscous tensor, and $\boldsymbol{\mathcal{Q}}$ the heat flux.

A remarkable feature of dissipative plasmas is the anisotropy of the transport fluxes under strong magnetic fields [12, 49]. We denote by $\boldsymbol{\mathcal{B}}$ the unitary vector $\boldsymbol{\mathcal{B}} = \boldsymbol{B}/B$, where $B = \|\boldsymbol{B}\|$, and for any vector $\mathbf{x}$ of $\mathbb{R}^3$, we may consider the three associated vectors $\mathbf{x}^{\parallel} = (\boldsymbol{\mathcal{B}}\boldsymbol{\cdot}\mathbf{x})\boldsymbol{\mathcal{B}}$, $\mathbf{x}^{\perp} = \mathbf{x} - \mathbf{x}^{\parallel}$ and $\mathbf{x}^{\odot} = \boldsymbol{\mathcal{B}}\wedge\mathbf{x}$, which are orthogonal. The species diffusion velocities $\boldsymbol{V}_k$, $k \in S$, can then be written

$$\begin{aligned}\boldsymbol{V}_k = -\sum_{l\in S} \big(D_{kl}^{\parallel}\boldsymbol{d}_l^{\parallel} + D_{kl}^{\perp}\boldsymbol{d}_l^{\perp} + D_{kl}^{\odot}\boldsymbol{d}_l^{\odot}\big)&\\ - \big(\theta_k^{\parallel}(\partial_x \mathrm{log}T)^{\parallel} + \theta_k^{\perp}(\partial_x \mathrm{log}T)^{\perp} + \theta_k^{\odot}(\partial_x \mathrm{log}T)^{\odot}\big)&,\end{aligned} \tag{6.6}$$

where the diffusion driving forces $\boldsymbol{d}_k$, $k \in S$, are given by

$$\boldsymbol{d}_k = \tfrac{1}{p}\big(\partial_x p_k - q_k(\boldsymbol{E} + \boldsymbol{v}\wedge\boldsymbol{B})\big), \tag{6.7}$$

and $D_{kl}^{\parallel}$, $D_{kl}^{\perp}$, and $D_{kl}^{\odot}$, $k, l \in S$, are the multicomponent diffusion coefficients, $\theta_k^{\parallel}$, $\theta_k^{\perp}$, and $\theta_k^{\odot}$, $k \in S$, the thermal diffusion coefficients, T the absolute temperature, p_k, $k \in S$, the species partial pressures. The heat flux $\boldsymbol{\mathcal{Q}}$ can be written

$$\begin{aligned}\boldsymbol{\mathcal{Q}} = -\widehat{\lambda}^{\parallel}(\partial_x T)^{\parallel} - \widehat{\lambda}^{\perp}(\partial_x T)^{\perp} - \widehat{\lambda}^{\odot}(\partial_x T)^{\odot}&\\ - p\sum_{k\in S}\big(\theta_k^{\parallel}\boldsymbol{d}_k^{\parallel} + \theta_k^{\perp}\boldsymbol{d}_k^{\perp} + \theta_k^{\odot}\boldsymbol{d}_k^{\odot}\big) + \sum_{k\in S} \rho_k h_k \boldsymbol{V}_k&,\end{aligned} \tag{6.8}$$

where h_k, $k \in S$, are the species enthalpy per unit mass, and $\widehat{\lambda}^{\parallel}$, $\widehat{\lambda}^{\perp}$, and $\widehat{\lambda}^{\odot}$ the partial thermal conductivities. Finally, the viscous tensor $\boldsymbol{\Pi}$ is given by

$$\begin{aligned}\boldsymbol{\Pi} = -\kappa(\partial_x\cdot\boldsymbol{v})\boldsymbol{I} - \eta_1\mathsf{S} - \eta_2(\boldsymbol{M}^{\odot}\mathsf{S} - \mathsf{S}\boldsymbol{M}^{\odot}) - \eta_3(-\boldsymbol{M}^{\odot}\mathsf{S}\boldsymbol{M}^{\odot} + \boldsymbol{M}^{\parallel}\,\mathsf{S}\,\boldsymbol{M}^{\parallel}) \\ - \eta_4(\mathsf{S}\,\boldsymbol{M}^{\parallel} + \boldsymbol{M}^{\parallel}\,\mathsf{S} - 2\boldsymbol{M}^{\parallel}\,\mathsf{S}\,\boldsymbol{M}^{\parallel}) - \eta_5(\boldsymbol{M}^{\parallel}\,\mathsf{S}\,\boldsymbol{M}^{\odot} - \boldsymbol{M}^{\odot}\,\mathsf{S}\,\boldsymbol{M}^{\parallel}),\end{aligned} \tag{6.9}$$

where κ is the volume viscosity, η_1, η_2, η_3, η_4, and η_5, the shear viscosities. We have denoted by S the symmetric traceless deformation rate tensor

$$\mathsf{S} = \partial_x\boldsymbol{v} + \partial_x\boldsymbol{v}^t - \tfrac{2}{3}(\partial_x\cdot\boldsymbol{v})\boldsymbol{I},$$

by $\boldsymbol{M}^{\parallel}$ the matrix $\boldsymbol{M}^{\parallel} = \boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}}$ and by $\boldsymbol{M}^{\odot}$ the antisymmetric rotation matrix associated with the vector $\boldsymbol{\mathcal{B}}$

$$\boldsymbol{M}^{\odot} = \begin{pmatrix} 0 & -\mathcal{B}_3 & \mathcal{B}_2 \\ \mathcal{B}_3 & 0 & -\mathcal{B}_1 \\ -\mathcal{B}_2 & \mathcal{B}_1 & 0 \end{pmatrix}.$$

These fluxes $\boldsymbol{V}_k$, $k \in S$, $\boldsymbol{\Pi}$, and $\boldsymbol{Q}$ are smooth functions of $\boldsymbol{B}$ thanks to the structural properties of the multicomponent transport coefficients parallel, orthogonal, and transverse to the magnetic field $\boldsymbol{B}$ deduced from the kinetic theory [24].

The convective fluxes $\mathcal{F}_i(U)$, $i \in C$, are $\mathcal{C}^\infty$ functions of the variable $U \in \mathcal{O}_U$, where $\mathcal{O}_U$ is a convex open set of $\mathbb{R}^{\mathsf{n}}$ where $\mathsf{n} = n + 10$, and the dissipative fluxes $\mathcal{F}_i^{\mathrm{diss}}(U, \partial_x U)$, $i \in C$, can be written in the form

$$\mathcal{F}_i^{\mathrm{diss}}(U, \partial_x U) = -\sum_{j\in C} B_{ij}(U)\big(\partial_j U + G_j(U)\big), \qquad i \in C, \tag{6.10}$$

where the dissipation matrices $B_{ij}(U)$, $i, j \in C$, and the zeroth order contributions $G_i(U)$, $i \in C$, are $\mathcal{C}^\infty$ functions of $U \in \mathcal{O}_U$. In addition, the source term $\Omega^{\boldsymbol{j}}(U, \partial_x U)$ can be written in the form

$$\Omega^{\boldsymbol{j}}(U, \partial_x U) = \sum_{i\in C} M_i(U)^t\ \mathcal{F}_i^{\mathrm{diss}}(U, \partial_x U) + \Omega_0(U), \tag{6.11}$$

where the matrices $M_i(U)$, $i \in C$, and the zeroth order source term $\Omega_0(U)$ are $\mathcal{C}^\infty$ functions of $U \in \mathcal{O}_U$.

The dissipative terms $\mathcal{F}_i^{\mathrm{diss}}$, $i \in C$, notably contain the zeroth-order contributions G_i, $i \in C$, arising from the direct action of electromagnetic forces. Another difference with nonionized mixtures is that the source term $\Omega^{\boldsymbol{j}}$ also depends on the gradient $\partial_x U$ through the current $\boldsymbol{j}$ appearing in Maxwell's equations and these terms are related through entropy. Finally, denoting by $A_i(U) = \partial_U \mathcal{F}_i$, $i \in C$, the Jacobian matrices, which are $\mathcal{C}^\infty$ functions of $U \in \mathcal{O}_U$, and the system (6.1) can be rewritten in the form

$$\begin{aligned}\partial_t U + \sum_{i\in C} A_i(U)\partial_i U = \sum_{i,j\in C} \partial_i\Big(B_{ij}(U)\big(\partial_j U + G_j(U)\big)\Big) \\ - \sum_{i,j\in C} M_i(U)^t B_{ij}(U)\big(\partial_j U + G_j(U)\big) + \Omega_0(U).\end{aligned} \tag{6.12}$$

Remark 6.1. *Denoting by m_{e} the electron mass, the singular limit $m_{\mathrm{e}} \to 0$ is not addressed in these notes. In the limit $m_{\mathrm{e}} \to 0$, anisotropy is lost excepted for electrons, and we refer to [52] for more details.*

6.2 Symmetrization and normal form

The mathematical entropy σ is taken to be the opposite of the physical entropy per unit volume $\sigma = -\mathcal{S}$ and is a $\mathcal{C}^\infty$ strictly convex function of $U \in \mathcal{O}_U$. The corresponding vector of entropic variables $V = (\partial_U \sigma)^t$ is given by

$$V = \tfrac{1}{T}\Big(g_1 - \tfrac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v}, \ldots, g_n - \tfrac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v},\ \boldsymbol{v},\ \varepsilon_0\boldsymbol{E},\ \boldsymbol{B}/\mu_0,\ -1\Big)^t, \tag{6.13}$$

where g_k, $k \in S$, are the species Gibbs functions.

Theorem 6.2. *Performing the change of variable $U = U(V)$, the system* (6.12) *is transformed into*

$$\widetilde{A}_0(V)\,\partial_t V + \sum_{i\in C}\widetilde{A}_i(V)\partial_i V = \sum_{i,j\in C}\partial_i\Big(\widetilde{B}_{ij}(V)\big(\partial_j V + \widetilde{G}_j(V)\big)\Big)$$
$$- \sum_{i,j\in C}\widetilde{M}_i(V)^t\,\widetilde{B}_{ij}(V)\big(\partial_j V + \widetilde{G}_j(V)\big) + \widetilde{\Omega}_0(V), \tag{6.14}$$

with $\widetilde{A}_0 = \partial_V U$, $\widetilde{A}_i = A_i\partial_V U$, $\widetilde{B}_{ij} = \widetilde{B}^{\rm s}_{ij} + \widetilde{B}^{\rm a}_{ij} = B_{ij}\partial_V U$, $\widetilde{G}_i = (\partial_V U)^{-1}G_i$, $\widetilde{M}_i = M_i$ and $\widetilde{\Omega}_0 = \Omega_0$, where the matrices $\widetilde{A}_0(V)$, $\widetilde{A}_i(V)$, $\widetilde{M}_i(V)$, $i \in C$, $\widetilde{B}^{\rm s}_{ij}(V)$, $\widetilde{B}^{\rm a}_{ij}(V)$, $i, j \in C$, and the vectors $\widetilde{G}_i(V)$, $i \in C$, $\widetilde{\Omega}_0(V)$ are $\mathcal{C}^\infty$ functions of $V \in \mathcal{O}_V$, where $\mathcal{O}_V$ is a convex open of $\mathbb{R}^{\mathsf{n}}$.

Furthermore, the system (6.14) *is in partially the symmetric form, that is, the matrix $\widetilde{A}_0(V)$ is symmetric positive definite, the matrices $\widetilde{A}_i(V)$, $i \in C$, are symmetric, we have the relations $\widetilde{B}^{\rm s}_{ij}(V)^t = \widetilde{B}^{\rm s}_{ji}(V)$, $\widetilde{B}^{\rm a}_{ij}(V)^t = -\widetilde{B}^{\rm a}_{ji}(V)$, $i, j \in C$, the matrix $\widetilde{B}(V, \boldsymbol{\xi}) = \sum_{i,j\in C}\widetilde{B}^{\rm s}_{ij}(V)\xi_i\xi_j$ is symmetric positive semi-definite for $\boldsymbol{\xi} \in \Sigma^2$, where Σ^2 is the unit sphere of $\mathbb{R}^3$, and $V \in \mathcal{O}_V$. For x in the nullspace of $N(\widetilde{B})$, we have $\widetilde{B}^{\rm s}_{ij}x = 0$ and $\widetilde{B}^{\rm a}_{ij}x = 0$, $i, j \in C$, and the compatibility relations $\widetilde{G}_i(V) = \widetilde{M}_i(V)V$, $i \in C$, are satisfied.*

The corresponding new definition of entropy is given in [51] with the associated equivalence theorem. The equation governing the entropy is easily obtained upon multiplying on the left equation (6.14) by V^t and can be written

$$\partial_t\sigma + \sum_{i\in C}\partial_i\mathfrak{q}_i + \sum_{i\in C}\partial_i\mathfrak{p}_i = -\sum_{i,j\in C}\langle\partial_i V + \widetilde{M}_i V, \widetilde{B}^{\rm s}_{ij}(\partial_i V + \widetilde{M}_i V)\rangle + \langle\widetilde{\Omega}_0, V\rangle, \tag{6.15}$$

where $\mathfrak{q}_i$, $i \in C$, are the convective entropy fluxes, $\mathfrak{p}_i$, $i \in C$, the dissipative entropy fluxes associated to dissipative effects in the $i^{\rm e}$ direction, $\mathfrak{p}_i = \langle V, F_i^{\rm diss}\rangle$. It is important to observe that the zeroth order contributions are included in the entropy production term [49, 51] and that only the symmetric parts of the dissipation matrices $\widetilde{B}^{\rm s}_{ij}$ play a rôle in this source term.

We next rewrite the symmetric system (6.14) by regrouping all the zeroth order terms as a source and next all first order derivatives arising from the zeroth order contributions of dissipative fluxes as well as from the gradient dependent source terms with the convective terms. To this aim, we define the new matrices $\widetilde{A}^{\rm a}_i$, $i \in C$, and the new source $\widetilde{\Omega}$ by

$$\widetilde{A}^{\rm a}_i(V) = \sum_{j\in C}\big(\widetilde{M}^t_j\,\widetilde{B}_{ji} - \widetilde{B}_{ij}\widetilde{M}_j - \partial_V(\widetilde{B}_{ij}\widetilde{M}_j)V\big),$$
$$\widetilde{\Omega}(V) = -\sum_{i,j\in C}\widetilde{M}^t_i\widetilde{B}_{ij}\widetilde{M}_j V + \widetilde{\Omega}_0(V).$$

The resulting symmetric system is still intermediate between a symmetric hyperbolic system and a symmetric strongly parabolic system. In order to rewrite this system into a partially normal form, we investigate the nullspace invariance property.

Proposition 6.3. *The nullspace N of the symmetric matrix*

$$\widetilde{B}(V, \boldsymbol{\xi}) = \sum_{i,j\in C}\widetilde{B}^{\rm s}_{ij}(V)\xi_i\xi_j,$$

does not depends on $V \in \mathcal{O}_V$ or $\boldsymbol{\xi} \in \Sigma^2$. This nullspace of dimension 7 is spanned by the column vectors $(1, \ldots, 1, 0_{1,10})^t$ and e^{n+k}, $k = 1, \ldots, 6$, where $(\mathsf{e}^k)_{k=1,\ldots,n+10}$ is the canonical basis of $\mathbb{R}^{n+10}$.

In order to separate hyperbolic and parabolic variables, we introduce the partially normal variables $W = (W_{I}, W_{II})^t$ where W_{I} corresponds to the hyperbolic variables and W_{II} to the parabolic variables

$$W_{I} = \big(\rho, \boldsymbol{E}, \boldsymbol{B}\big)^t, \qquad W_{II} = \big(\log(\rho_2^{r_2}/\rho_1^{r_1}), \ldots, \log(\rho_n^{r_n}/\rho_1^{r_1}), \boldsymbol{v}, T\big)^t. \tag{6.16}$$

The system of dissipative plasmas can now be recast into a partially normal form, that is to say into a partially symmetric hyperbolic-parabolic composite form. We use the term partially symmetric since the resulting effective first order differential operators involve nonsymmetric matrices in contrast with the nonionized case [7, 15, 18, 21]. However, the bloc structure of the additional first order differential operators insures that the symmetric properties concerning the hyperbolic subsystem are conserved [51].

Proposition 6.4. *Performing the change of variable $V = V(W)$, the system (6.14) is transformed into*

$$\begin{aligned}\overline{A}_0(W)\partial_t W + \sum_{i\in C}\big(\overline{A}_i(W)+\overline{A}_i^{\mathrm{a}}(W)\big)\partial_i W = \\ \sum_{i,j\in C}\partial_i\Big(\overline{B}_{ij}(W)\partial_j W\Big) + \overline{\mathcal{T}}(W,\partial_x W) + \overline{\Omega}(W),\end{aligned} \tag{6.17}$$

where we have defined $\overline{A}_0 = (\partial_W V)^t\,\widetilde{A}_0\,(\partial_W V)$, $\overline{A}_i = (\partial_W V)^t\,\widetilde{A}_i\,(\partial_W V)$ and $\overline{A}_i^{\mathrm{a}} = (\partial_W V)^t\,\widetilde{A}_i^{\mathrm{a}}\,(\partial_W V)$, $i \in C$, $\overline{B}_{ij} = (\partial_W V)^t\,\widetilde{B}_{ij}\,(\partial_W V)$, $i,j \in C$, $\overline{\Omega} = (\partial_W V)^t\,\widetilde{\Omega}$, $\overline{\mathcal{T}} = -\sum_{i,j\in C}\partial_i(\partial_W V)^t\,\widetilde{B}_{ij}\,(\partial_W V)\,\partial_j W$, and where the matrices $\overline{A}_0(W)$, $\overline{A}_i(W)$, $\overline{A}_i^{\mathrm{a}}(W)$, $i \in C$, $\overline{B}_{ij}(W)$, $i,j \in C$, and the vectors $\overline{\Omega}(W)$, $\overline{\mathcal{T}}(W,\partial_x W)$ are $\mathcal{C}^\infty$ functions of $W \in \mathcal{O}_W$ and $\partial_x W \in \mathbb{R}^{3n}$. Moreover, the system (6.17) is in partially normal form, that is, the matrix $\overline{A}_0(W)$ is symmetric positive definite, the matrices $\overline{A}_i(W)$ are symmetric, the matrices $\overline{A}_0$, $\overline{A}_i^{\mathrm{a}}$, $i \in C$, and $\overline{B}_{ij}$, $i,j \in C$, have the block structure

$$\overline{A}_0 = \begin{pmatrix}\overline{A}_0^{\mathrm{I,I}} & 0\\ 0 & \overline{A}_0^{\mathrm{II,II}}\end{pmatrix}, \quad \overline{A}_i^{\mathrm{a}} = \begin{pmatrix}0 & \overline{A}_i^{\mathrm{aI,II}}\\ \overline{A}_i^{\mathrm{aII,I}} & \overline{A}_i^{\mathrm{aII,II}}\end{pmatrix}, \quad \overline{B}_{ij} = \begin{pmatrix}0 & 0\\ 0 & \overline{B}_{ij}^{\mathrm{II,II}}\end{pmatrix},$$

the matrix $\overline{B}^{\mathrm{II,II}}(W,\boldsymbol{\xi}) = \sum_{i,j\in C}\overline{B}_{ij}^{\mathrm{II,II}}(W)\xi_i\xi_j$ is such that $\mathsf{X}^t\;\overline{B}(W,\boldsymbol{\xi})\;\mathsf{X} > 0$, for $\mathsf{X} \in \mathbb{R}^{\mathsf{n}-7}$, $\mathsf{X} \neq 0$, $\boldsymbol{\xi} \in \Sigma^2$ and $W \in \mathcal{O}_W$ and we have $\overline{\mathcal{T}}(W,\partial_x W) = \big(\overline{\mathcal{T}}_{\mathrm{I}}(W,\partial_x W_{II}),\overline{\mathcal{T}}_{\mathrm{II}}(W,\partial_x W)\big)^t$.

6.3 Local existence theorem

We may now investigate the well posedness of the Cauchy problem by using a simplified quasilinear version of an existence theorem due to Vol'pert and Hudjaev [14, 21, 51] concerning partially symmetric hyperbolic-parabolic systems.

We introduce the Vol'Pert's functional spaces $V_l(\mathbb{R}^3)$ with norm

$$\|\phi\|_{V_l}^2 = \sum_{i\in[\![1,n]\!]}\|\phi_i\|_{V_l}^2, \qquad \|\phi_i\|_{V_l} = \|\phi_i\|_{L^\infty} + \sum_{k\in[\![1,l]\!]}|\phi_i|_{H^k}, \tag{6.18}$$

where $\phi = (\phi_1,\dots,\phi_n)^t$ and $|\phi_i|_{H^k} = \|\partial_x^k\phi_i\|_{L^2}$ denotes the usual seminorm associated with the Sobolev space H^k. The solutions are investigated in the space $V_l(\mathbb{R}^3)$ where l is an integer greater than $9/2$.

Using the partially normal form obtained previously, we may now prove local existence and uniqueness in the space $V_l(\mathbb{R}^3)$ for the Cauchy problem (6.17) with an initial condition $W^0 \in V_l(\mathbb{R}^3)$ such that $\inf_{\mathbb{R}^3}\rho^0 > 0$ and $\inf_{\mathbb{R}^3}T^0 > 0$. Moreover, the solution is continuous with its derivatives of first order in t and second order in x.

Theorem 6.5. *Consider the Cauchy problem for the system (6.17) in $\mathbb{R}^3$ with initial conditions $W(0,x) = W^0(x)$, $x \in \mathbb{R}^3$, where $W^0 \in V_l(\mathbb{R}^3)$, $l > 9/2$, $\inf_{\mathbb{R}^3}\rho^0 > 0$ and $\inf_{\mathbb{R}^3}T^0 > 0$. There exists $t_0 > 0$, such that the Cauchy problem admits a unique solution $W = (W_I, W_{II})^t$ with $W(t,x) \in \mathcal{O}_W$, defined on the domain $\overline{Q}_{t_0} = [0,t_0]\times\mathbb{R}^3$, which is continuous in $\overline{Q}_{t_0}$ as well as its derivatives of first order in t and second order in x and the following quantities remain finite*

$$\sup_{0\leqslant t\leqslant t_0}\|(W_I(t),W_{II}(t))\|_{V_l}, \qquad \sup_{\overline{Q}_{t_0}}(1/\rho+1/T), \qquad \sup_{0\leqslant t\leqslant t_0}\|\partial_t W_I(t)\|_{V_{l-1}},$$

$$\int_0^{t_0}\big(\|\partial_t W_{II}(\tau)\|_{V_{l-1}}^2+\|W_{II}(\tau)\|_{V_{l+1}}^2\big)\mathrm{d}\tau.$$

In addition, either t_0 can be taken arbitrary large, or there exists t_1 such that the theorem is true for $t_0 < t_1$ but as $t_0 \to t_1^-$, at least one of the quantities $\|W_I(t_0)\|_{W^{1,\infty}} + \|W_{II}(t_0)\|_{W^{2,\infty}}$ and $\sup_{\overline{Q}_{t_0}} 1/T$ is unbounded.

Note that the partially normal form obtained for dissipative plasmas is insufficient in order to establish global existence results around constant equilibrium states [7, 15, 20]. More specifically, consider an equilibrium state W^{e} such $\boldsymbol{E}^{\mathrm{e}} = \boldsymbol{B}^{\mathrm{e}} = \boldsymbol{v}^{\mathrm{e}} = 0$. One can establish that the matrices $\overline{A}_i^{\mathrm{ae}}$, $i \in C$, are antisymmetric and never vanish, so that we cannot apply the existence theorem established in [15, 20, 7]. These theorems may still be used in the ambipolar limit. The ambipolar approximation is a model for ionized reactive gas mixtures obtained for vanishing Debye length for which the asymptotic stability around constant equilibrium states is established in [24]. The ambipolar model is also stable when the electron mass goes to zero [24].

7 Numerical simulation

Numerical simulation of multicomponent reactive flows with complex chemistry and detailed transport phenomena is of fundamental important for many engineering applications. We briefly discuss in this section some numerical algorithms specially devoted to multicomponent flows.

7.1 Numerical Methods

Numerical simulation of compressible flows is a very difficult task that has been the subject of numerous textbooks and requires a solid background in fluid mechanics and numerical analysis [55, 57, 59]. The nature of compressible flows may be very complex, with features such as shock fronts, boundary layers, turbulence, acoustic waves, or instabilities. Taking into account chemical reactions dramatically increases the difficulties, especially when detailed chemical and transport models are considered. Interactions between chemistry and fluid mechanics are especially complex in reentry problems [1], combustion phenomena [5, 60, 62], or chemical vapor deposition reactors [3, 4].

An important aspect of complex chemistry flows is the presence of multiple time scales. For compressible flows, we already know that the presence of acoustic waves introduces small characteristic times for small Mach number flows. However, chemical characteristic times can range typically from 10^{-10} s up to several seconds. In the presence of multiple time scales, implicit methods are advantageous, since otherwise explicit schemes are limited by the smallest time scale [7, 55].

A second potential difficulty associated with the multicomponent aspect is the presence of multiple space scales. In combustion applications, for instance, the flame fronts are very thin and typically require space steps of 10^{-3} cm at atmospheric pressure, and even 10^{-5} cm at 100 atm, whereas a typical flow scale may be of 10 cm or even 100 cm. The multiple scales can only be solved by using adaptive grids obtained by successive refinements or by moving grids for unsteady problems [54, 55, 57, 58, 59, 60, 62].

Nonlinear discrete equations can be solved by using Newton's method or any generalization. The resulting large sparse linear systems must then be solved by using a Krylov-type method, such as GMRES [56]. More sophisticated methods involve coupled Newton–Krylov techniques [58]. Evaluating aerothermochemistry quantities is computationally expensive since they involve multiple sums and products. Optimal evaluation requires a low-level parallelization depending on the problem granularity.

Finally, it is preferable, when writing numerical software, to clearly separate the numerical tools from the special type of equations that are under concern. In the context of multicomponent flows, it is therefore a good idea to write codes for general mixtures and use libraries that automatically evaluate thermochemistry properties and transport properties. The evaluation of transport coefficients in multicomponent mixtures is discussed in the next section.

7.2 Transport coefficients

In order to evaluate the multicomponent transport coefficients given by the kinetic theory of gases, it is necessary to solve transport linear systems arising from the Chapman-Enskog procedure. The Chapman-Enskog method indeed requires solving systems of linearized integral Boltzmann equations with constraints through a Galerkin variational procedure. Various variational approximation spaces can be used as reduced spaces [13] or spaces for a direct evaluation of the thermal conductivity and the thermal diffusion ratios [66] and lead to different linear systems. The resulting transport linear systems are also naturally obtained in their symmetric form [8, 9, 11, 12, 13]. The linear system associated with any coefficient μ then take on either a regular form or a singular form [13, 7]. The singular form can be written in the general form

$$\begin{cases} G\alpha = \beta, \\ \langle \mathcal{G}, \alpha \rangle = 0, \end{cases} \tag{7.1}$$

where $G \in \mathbb{R}^{\omega,\omega}$, $\alpha, \beta, \mathcal{G} \in \mathbb{R}^{\omega}$, ω is the dimension of the variational space and the coefficient is obtained with a scalar product $\mu = \langle \alpha, \beta' \rangle$ [12, 13]. The matrix G is symmetric positive semi-definite, its nullspace is one dimensional $N(G) = \mathbb{R}\mathcal{N}$, $\beta \in R(G)$, and the well posedness condition $N(G) \oplus \mathcal{G}^{\perp} = \mathbb{R}^{\omega}$ holds [13]. The sparse transport matrix $db(G)$ is a submatrix [13] composed of diagonals of blocks of G, and $2db(G) - G$ and $db(G)$ are symmetric positive definite for $n \geq 3$. All these properties can rigorously be deduced from the properties of the Boltzmann linearized collision operator and that of the variational approximation spaces [13].

The solution of the transport linear system can then be obtained either from the symmetric positive definite system $(G + \mathcal{G} \otimes \mathcal{G})\alpha = \beta$ or from iterative techniques. The iterative techniques are either generalized conjugate gradients or stationary techniques associated with a splitting $G = M - W$, $M = db(G)$, and yield

$$\alpha = \sum_{0 \leq j < \infty} (PT)^j P M^{-1} P^t \beta, \tag{7.2}$$

where $T = M^{-1}W$ and $P = I - \mathcal{N} \otimes \mathcal{G} / \langle \mathcal{N}, \mathcal{G} \rangle$. The matrix $M + W = 2db(G) - G$ must be positive definite but this is a consequence from Boltzmann linearized equations. These stationary and generalized conjugate gradients methods have been found to be efficient for mixture of neutral gases [5, 65, 66, 67, 68, 69].

The situation of ionized mixtures is more complex since the convergence rate of stationary iterative techniques deteriorate as the ionization level increases as discovered by García Muñoz [70]. On the contrary, the convergence properties of generalized conjugate gradient algorithms do not depend on the ionization level. New algorithms have been thus been introduced with *more singular* versions of the transport linear systems. These algorithms have led to fast convergence rates for all ionization levels and magnetic field intensities [71].

7.3 Impact of multicomponent transport

Recent numerical investigations have brought further support for the importance of accurate transport property in various multicomponent reactive flows. Thermal diffusion effects have been shown to be important in the study of vortex-flame interaction [75], catalytic effects near walls, interfacial phenomena, gaseous or spray diffusion flames [76, 79, 80], and chemical vapor deposition reactors [4]. The impact of multicomponent diffusion has also been shown to be important in multidimensional hydrogen/air and methane/air Bunsen flames [5], in freely propagating flames—especially with oxygen as pure oxydizer—as well as in direct numerical simulation of turbulent flames [77]

As a typical exemple, we consider a lean hydrogen-air Bunsen flame obtained by flowing a lean mixture of 20% hydrogen in air at 300 K and at atmospheric pressure through a cylindrical tube [7]. When the exit velocity exceeds the planar flame speed, these flames are of conical shape and sit at the mouth of the cylindrical burner. The tube inner diameter is $r_i = 4$ mm, the tube width is $w = 0.5$ mm, and the burner temperature is kept at 300 K. The flow is of plug type, and the flame is surrounded by a coflow of air. The maximum velocity in both flows is $v_{\rm inj} = 300$ cm/sec and we refer to [7] for more details. The computational domain is [0,1.5]×[0,30] in centimeters and approximately 200 points are adaptively distributed in each direction. The governing equations are obtained from the fundamental equations presented in Section 2 specialized to the steady axisymmetric setting.

We have used the chemical reaction mechanism is presented in Table 1. This reaction mechanism describe the combustion of hydrogen in air and involves the $n = 9$ species H, O, H_2, O_2, N_2, OH, HO_2, H_2O, and H_2O_2. Taking into account the shortcut of using the third body M, which denotes any species of the mixture, this reaction mechanism involve $n^{\rm r} = 57$ elementary reversible reactions.

Figure 1 presents the atomic oxygen radical O mole fraction distribution around the tube rim and the plotting domain is $[0.5, 0.5] \times [0, 1]$ in cm. The right-hand side of the plot presents the numerical solution with thermal diffusion neglected and the left-hand side the corresponding values obtained with thermal diffusion effects. In Figure 1 the light species O tends to stay in hotter zones when thermal diffusion effects are taken into account.

Finally, theoretical calculations and experimental measurements have also shown that the ratio κ/η is not small for polyatomic gases. Volume viscosity also arises in dense gases and in liquids, and its absence in dilute monatomic gases is an exception rather than a rule. Despite its potential importance, volume or bulk viscosity has seldom been included in computational models of multidimensional reactive

Table 1: Warnatz kinetics scheme for hydrogen combustion [72]

i	Reaction	$\mathfrak{A}_i$	$\mathfrak{b}_i$	$\mathfrak{E}_i$
1	$H + O_2 \leftrightarrows OH + O$	2.00E+14	0.00	16802.
2	$O + H_2 \leftrightarrows OH + H$	5.06E+04	2.67	6286.
3	$OH + H_2 \leftrightarrows H_2O + H$	1.00E+08	1.60	3298.
4	$2OH \leftrightarrows O + H_2O$	1.50E+09	1.14	100.
5	$H + H + M \leftrightarrows H_2 + M^a$	6.30E+17	-1.00	0.
6	$H + OH + M \leftrightarrows H_2O + M^a$	7.70E+21	-2.00	0.
7	$O + O + M \leftrightarrows O_2 + M^a$	1.00E+17	-1.00	0.
8	$H + O_2 + M \leftrightarrows HO_2 + M^a$	8.05E+17	-0.80	0.
9	$H + HO_2 \leftrightarrows 2OH$	1.50E+14	0.00	1004.
10	$H + HO_2 \leftrightarrows H_2 + O_2$	2.50E+13	0.00	693.
11	$H + HO_2 \leftrightarrows H_2O + O$	3.00E+13	0.00	1721.
12	$O + HO_2 \leftrightarrows O_2 + OH$	1.80E+13	0.00	-406.
13	$OH + HO_2 \leftrightarrows H_2O + O_2$	6.00E+13	0.00	0.
14	$HO_2 + HO_2 \leftrightarrows H_2O_2 + O_2$	2.50E+11	0.00	-1242.
15	$OH + OH + M \leftrightarrows H_2O_2 + M^a$	1.14E+22	-2.00	0.
16	$H_2O_2 + H \leftrightarrows HO_2 + H_2$	1.70E+12	0.00	3752.
17	$H_2O_2 + H \leftrightarrows H_2O + OH$	1.00E+13	0.00	3585.
18	$H_2O_2 + O \leftrightarrows HO_2 + OH$	2.80E+13	0.00	6405.
19	$H_2O_2 + OH \leftrightarrows H_2O + HO_2$	5.40E+12	0.00	1004.

[a] Third body efficiency $H_2 = 2.86$, $N_2 = 1.43$, $H_2O = 18.6$
Units are moles, centimeters, seconds, calories, and Kelvins

flows. For small Mach number flows, however, the whole term $\boldsymbol{\partial}_x\cdot\big(\kappa(\boldsymbol{\partial}_x\cdot\boldsymbol{v})I\big)$ has a weak influence because of its *structure*, even though both the ratio κ/η and the dilatation $\boldsymbol{\partial}_x\cdot\boldsymbol{v}$ may not be small [7]. However, it has been shown that volume viscosity has an important impact during a shock/hydrogen bubble interaction [78].

8 Conclusion and future directions

The models developed in the previous sections may be used to describe gas mixtures in full vibrational nonequilibrium when each vibrational quantum level is treated as a separate "chemical species" allowing detailed state-to-state relaxation models [21]. When the vibrational quantum levels are partially at equilibrium between them but not at equilibrium with the translational/rotational states—allowing the definition of a vibrational temperature—a different structure is obtained.

The mathematical analysis of chemical equilibrium flows has recently be extended to the situation of partial chemical equilibrium [48]. However, the mathematical structure of numerous simplified chemistry methods is still obscure from a mathematical point of view at variance with partial equilibrium.

Various extensions could also consider initial-boundary value problems [81] with the possibility of inflow or outflow conditions, heat losses, or surface reactions with complex heterogeneous chemistry. Multicomponent reactive flows with radiative transfer [32] should also be investigated [27]. Various numerical analysis theoretical results could also be extended to the case of mixtures like convergence results of Petrov-Galerkin 'Streamline–Diffusion' finite element techniques [63, 82].

The notion of higher order entropy may also be generalized to the situation of multicomponent flows [83, 84, 85] as well as the singular limit of small Mach number flow [86, 87]. Multiphase flows with sprays governed by Boltzmann type equations [32], or derived multifluid sectional models for droplets [88], may also be investigated mathematically.

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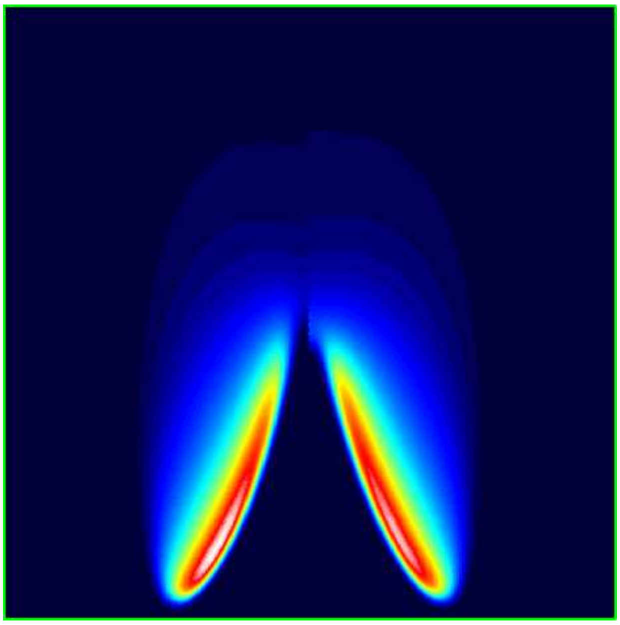

Figure 1: Atomic oxygen radical mole fraction in a Hydrogen/Air Bunsen laminar flame. Soret effect is neglected of the right and included on the left hand side of the picture.

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