

MULTICOMPONENT MODELS IN NUCLEAR ASTROPHYSICS

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Abstract. We consider hydrodynamical models describing the evolution of a gaseous star in which the presence of thermonuclear reactions between several species leads to a multicomponent formulation. In the case of binary mixtures, recent 3D results are evoked. In the one-dimensional situation, we can prove global estimates and stabilization for some simplified model.

1. Introduction. Stars can generally be considered as continuous media for which hydrodynamical description is natural, then the equations governing the evolution of stellar structure are almost identical to those describing ordinary fluid mechanics [30] [38] [18], except the fact that, due to various chemical reactions taking place in the medium (more precisely thermonuclear reactions), one has to consider a multicomponent mixture containing several particle species.

Multifluids have been the matter of a number of works in the past which, for our purposes, may be very roughly divided into those concerning multiphase flows and those involving multicomponent flows. The first kind of models suppose that, given several fluids, only one of them is present into each given (“bubble” like) macroscopic region of space, each bubble being plugged into an underlying fluid region. One is then faced with a multifluid free boundary problem [36] [39] for each subregion (see [50] [46] [15] [31] [32] for related mathematical results).

In the multicomponent formulation [17] [33], each component is simultaneously present at any point of the space and global hydrodynamical variables for the mixture may be identified: the density, momentum, internal energy and entropy corresponding to a “mean flow” with suitable state functions, then dynamics is coupled to a reaction-diffusion system describing the evolution of the individual densities with source terms telling how

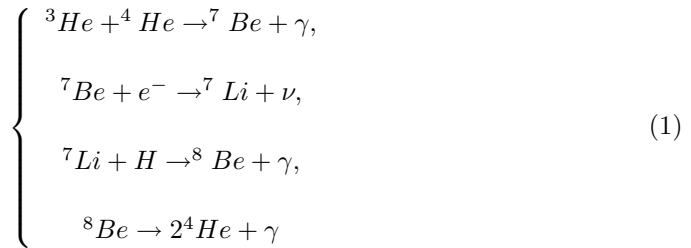
2000 *Mathematics Subject Classification*: Primary 76N10; Secondary 80A32.

Key words and phrases: multicomponent flow, binary mixture, gaseous star.

The paper is in final form and no version of it will be published elsewhere.

each species is produced (or destroyed) through chemical or thermonuclear reactions. Moreover the state functions depend now also on the individual concentrations. In the astrophysical setting, such reaction-diffusion systems lead to the chemical composition of stars [30].

Although multiphase flows may also be encountered in some astrophysical applications (models of plasma turbulence in stellar atmospheres [42]) we focus here on multicomponent flows involved in fundamental problems [38] [30] [44] as stellar evolution, nucleosynthesis or flows in interstellar medium which are presently actively studied by physicists. As an example of thermonuclear coupling in stars, let us only mention the so-called ‘‘PP II cycle’’ (Proton-Proton) describing describing the Helium chain in stellar nucleosynthesis [38] [30] [2]:



where He is helium, Be beryllium, Li lithium, H hydrogen, e^- an electron, ν a neutrino and γ a photon. In fact, a huge number of such cycles (leading from the lighter to the heavier nuclei) are present in stars and the competition between chemistry and gravitation is the core of stellar evolution.

In the following, we provide (section 2) a quick derivation of the multicomponent formulation, then (section 3) we present recent results of global existence for a simple model for binary mixtures finally we give in section 4 a stabilization result in the monodimensional case.

2. A general model. Let us start with a few words about multifluid systems, the description of which depends on the level of approximation one desires to assume.

In fact, the more precise way to deal with multifluids relies on kinetic theory [11] [8] leading to a complex Boltzmann formulation for the various distribution functions involved [7] [6].

This general framework allows to treat very out-of-equilibrium situations however, as we are interested in stellar evolution applications [30] [38], we restrict our study to the fluid regime for a mixture of N reacting species.

In fact, even the complete multicomponent fluid system evoked above is still too complex to lead to a complete analysis. As it modelizes various physical situations going from reacting astrophysical plasmas to chemical reactors or superfluids, it is natural to specialize it to the relevant physics involved. A major simplification takes place when the dynamics can be reduced to a one-fluid main (mean) flow, with source-flux couplings to the individual species. This indeed is the case in the reactive fluids case where a (possibly complex) chemical kinetics is coupled to the main flow, but this procedure requires some further modelling to get the state functions and the various fluxes.

Let us consider a mixture of N Newtonian fluids, each of which is characterized by the variables $\rho_i, \mathbf{u}_i, \theta_i$ with stress tensor $\sigma_i = -p_i \mathbf{I} + \pi_i \mathbf{u}_i$, where $p_i(\rho_i, \theta_i)$ is the pressure and $\pi_i(\mathbf{u}_i)$ is the viscous stress. We also suppose that a force \mathbf{f}_i acts at each point in i .

We define the global density of the mixture as

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

and the global velocity as

$$\rho \mathbf{u} := \sum_{i=1}^N \rho_i \mathbf{u}_i.$$

If we sum the partial continuity equations, we get first the familiar conservation law

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{2}$$

Now if we sum up the momentum equations and use the identity

$$\sum_{i=1}^N \rho_i \mathbf{u}_i \otimes \mathbf{u}_i = \rho \mathbf{u} \otimes \mathbf{u} + \sum_{i=1}^N \rho_i (\mathbf{u} - \mathbf{u}_i) \otimes (\mathbf{u} - \mathbf{u}_i),$$

we get formally a momentum-like conservation law

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \sigma + \mathbf{f},$$

where $\mathbf{f} := \sum_{i=1}^N \mathbf{f}_i$.

Now the effective stress tensor is

$$\sigma = \sum_{i=1}^N \{\sigma_i + \rho_i (\mathbf{u} - \mathbf{u}_i) \otimes (\mathbf{u} - \mathbf{u}_i)\} = \sum_{i=1}^N \{-p_i(\rho_i, \theta_i) \mathbf{I} + \pi_i + \rho_i (\mathbf{u} - \mathbf{u}_i) \otimes (\mathbf{u} - \mathbf{u}_i)\}.$$

Then, in order to obtain a mean flow system we can absorb the $(\mathbf{u} - \mathbf{u}_i)$ -quadratic term in this relation and make strong hypotheses on the partial stresses σ_i .

In the particular case of a one-temperature model and if all the species are perfect gas with the same constant $R_i = R$ i.e. $p_i(\rho_i, \theta_i) = R \rho_i \theta$, we get an effective pressure by applying the Dalton's law: the total pressure is the sum of the partial pressures

$$p(\rho, \theta) := \sum_{i=1}^N p_i(\rho_i, \theta),$$

however the viscous contribution

$$\pi := \sum_{i=1}^N \pi_i(\mathbf{u}_i),$$

cannot in general be expressed as a functional $\pi(\mathbf{u})$.

The same arguments applied to the energy equation lead to similar difficulties.

A way out is to discard the \mathbf{u}_i as dynamical variables and to define them by constitutive laws (a simple example of such is the Fick's diffusion law) in term of the temperature and the partial concentrations c_i , which amounts to suppose that although the species may diffuse in the mixture, they are dynamically advected by the mean flow only.

2.1. The equations for a multicomponent reacting mixture. In this section we adopt the notations of Giovangigli [34].

In the following model, we suppose that all the species are mutually in local thermodynamical equilibrium, including the radiative contribution. Then the problem involves a unique temperature field for all the species. We also suppose that the mixture is driven by a mean flow described by the macroscopic variables $(\rho, \mathbf{u}, \theta)$

We consider the mixture as a viscous compressible fluid with no source of mass, the the mass conservation of individual species reads

$$\partial_t(\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{u}) = w_i - \nabla \cdot \mathbf{J}_i, \quad (3)$$

for $i = 1 \dots N$, for the species mass fraction $Y_i = \frac{\rho_i}{\rho}$, where \mathbf{J}_i is the diffusion flux of the species i

$$\mathbf{J}_i = \rho Y_i \mathbf{v}_i,$$

where \mathbf{v}_i is the diffusion velocity of the species i , and w_i is the molar production rate for species i .

The species mass constraint (no global matter source) implies

$$\sum_{i=1}^N \mathbf{J}_i = 0, \quad \text{and} \quad \sum_{i=1}^N w_i = 0,$$

from which one gets the global mass conservation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (4)$$

Momentum conservation reads

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \sigma + \rho \sum_{i=1}^N Y_i \mathbf{f}_i, \quad (5)$$

with the species mass fraction $Y_i = \frac{\rho_i}{\rho}$. Energy conservation reads

$$\partial_t(\rho e) + \nabla \cdot (\rho e \mathbf{u}) = \sigma : \nabla \mathbf{u} - \nabla \cdot \mathbf{q} + \sum_{i=1}^N (\rho Y_i \mathbf{u} + \mathbf{J}_i) \cdot \mathbf{f}_i - \sum_{i=1}^N h_i w_i, \quad (6)$$

with $h_i = e_i + \frac{p_i}{\rho_i}$, where $e_i = e_i(\rho_i, \theta)$ and $p_i = p_i(\rho_i, \theta)$ define the thermodynamical state of the species i (with $\rho_i = \rho Y_i$). The stress tensor is assumed to be of the form

$$\sigma = -p(\rho, \theta, \{Y_i\}) \mathbf{1} + \mu \Delta \mathbf{u} + \nu \nabla(\operatorname{div} \mathbf{u}),$$

where the total pressure is given by the Dalton's law

$$p(\rho, \theta, \{Y_i\}) = \sum_{i=1}^N p_i(\rho, \theta, Y_i),$$

and the heat flux is

$$\mathbf{q} = -\lambda \nabla \theta + \sum_{i=1}^N h_i \mathbf{J}_i - p \sum_{i=1}^N D_{\theta, i} \mathbf{d}_i.$$

We consider the following diffusion model, generalizing the Fick's law, to fix the diffusion velocities

$$\mathbf{J}_i = \sum_{j=1}^N C_{ij} \mathbf{d}_j - \rho Y_i D_{\theta,i} \frac{\nabla \theta}{\theta},$$

where C_{ij} are the multicomponent flux diffusion coefficients, $D_{\theta,i}$ is the thermal diffusion coefficient and \mathbf{d}_j is the diffusion driving force \mathbf{d}_j given by

$$\mathbf{d}_j = \nabla X_j + (X_j - Y_j) \left(\frac{\nabla p}{p} \right) + \frac{\rho}{p} \sum_{k=1}^N Y_j Y_k (\mathbf{f}_j - \mathbf{f}_k),$$

where the mole fraction of the species i is

$$X_i = \frac{Y_i/W_i}{\sum_{k=1}^N Y_k/W_k}.$$

Finally let us suppose that the chemistry is described by a set of M reactions

$$\sum_{k=1}^N \nu'_{i,k} \mathcal{M}_i \rightarrow \sum_{k=1}^N \nu''_{i,k} \mathcal{M}_i \quad \text{for } k = 1 \dots M,$$

where $\nu'_{i,k}$ and $\nu''_{i,k}$ are the stoichiometric coefficients for species i , with chemical symbol \mathcal{M}_i appearing as a reactant and as a product, respectively.

The corresponding reaction rates w_i are given by different phenomenological expressions, depending on the physics involved.

In the combustion context chemical kinetics [51] using Arrhenius and mass action laws one takes generally

$$w_i = W_i \sum_{k=1}^M (\nu''_{i,k} - \nu'_{i,k}) B_k \theta^{\alpha_k} e^{-\frac{E_k}{R\theta}} \prod_{j=1}^N \left(\frac{\rho Y_j}{W_j} \right)^{\nu'_{j,k}} \quad \text{for } k = 1 \dots M.$$

In the astrophysical context [30]

$$w_i = -\mathcal{R}_i Y_i + \sum_{j=1}^N \mathcal{R}_{ij} Y_i Y_j + \sum_{k,l=1}^N \mathcal{R}_{kl} Y_k Y_l + \dots,$$

where $\mathcal{R}_i > 0$ characterizes the photodisintegrations (β -decays) of nucleus i , \mathcal{R}_{ab} is the rate, per unit of time and volume, of destruction (if $a = i$ or $b = i$) or production (if $a \neq i$ and $b \neq i$) of species i by a (two-body) nuclear reaction, and \dots is the contribution of N -body reactions with $N > 2$. All these coefficients are generally strongly dependent on ρ, θ .

Although a lot of its properties have been studied by Giovangigli [34], the previous system seems to be presently out of reach of mathematical treatment, at least concerning the reacting case. However, for a multicomponent model involving only thermodiffusion coupling, it is possible to prove a local existence result, extending the method of Tabata [49].

3. Simplified models for a binary mixture. We first consider, as a simple model, the first equation of the PP II cycle



We also suppose that the reaction takes place in the presence of neutrons acting as a dilutant, so this unique reaction ($M = 1$) implies $N = 4$ species (discarding the massless photons), and we suppose that the field force does not depend on the species $\mathbf{f}_i \equiv \mathbf{f} = -G\nabla\Phi$ (gravitation). The system reads

$$\left\{ \begin{array}{l} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f}, \\ \partial_t (\rho e) + \nabla \cdot (\rho e \mathbf{u}) = \sigma : \nabla \mathbf{u} - \nabla \cdot \mathbf{q} + \rho \mathbf{f} \cdot \mathbf{u} + \mathbf{f} \cdot \sum_{i=1}^N \mathbf{J}_i - \sum_{j=1}^4 h_j^0 w_j, \\ \partial_t (\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{u}) = w_i - \nabla \cdot \mathbf{J}_i, \end{array} \right. \quad (8)$$

for $i = {}^3\text{He}, {}^4\text{He}, {}^7\text{Be}, n$ (with $Y_{{}^3\text{He}} + Y_{{}^4\text{He}} + Y_{{}^7\text{Be}} + Y_n = 1$), where the fluxes are

$$\mathbf{J}_i = \sum_{j=1}^4 C_{ij} \mathbf{d}_j - \rho Y_i D_{\vartheta, i} \frac{\nabla \vartheta}{\theta},$$

where the last term corresponds to a diffusion arising from a temperature gradient (Soret effect), and

$$\begin{aligned} \mathbf{d}_j &= \nabla X_j + (X_j - Y_j) \frac{\nabla p}{p}, \\ \mathbf{q} &= -\lambda \nabla \vartheta + \sum_{i=1}^4 h_i \mathbf{J}_i - p \sum_{i=1}^4 D_{\theta, i} \mathbf{d}_i, \end{aligned}$$

where the last term corresponds to heat diffusion arising from a concentration gradient (Dufour effect).

The chemical source terms are

$$\left\{ \begin{array}{l} w_{{}^3\text{He}} = -W_{{}^3\text{He}} \Phi, \\ w_{{}^4\text{He}} = -W_{{}^4\text{He}} \Phi, \\ w_{{}^7\text{Be}} = W_{{}^7\text{Be}} \Phi, \end{array} \right.$$

where

$$\Phi := B \vartheta^\alpha e^{-\frac{E}{R^0 \vartheta}} \frac{\rho Y_{{}^3\text{He}}}{W_{{}^3\text{He}}} \frac{\rho Y_{{}^4\text{He}}}{W_{{}^4\text{He}}}.$$

If we neglect the Soret and Dufour effects and if we suppose $C_{ij} = C \delta_{ij}$, and that the species specific heats at constant pressure are constant and independent of temperature, we get for \mathbf{J}_i the pure Fick's law

$$\mathbf{J}_i = -\rho D_i \nabla Y_i,$$

where D_i is the empirical diffusion coefficient of species i and

$$\mathbf{q} = -\lambda \nabla \vartheta.$$

Then we get the system

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \sigma + \rho \mathbf{f}, \\ \partial_t (\rho e) + \nabla \cdot (\rho e \mathbf{u}) = \sigma : \nabla \mathbf{u} + \nabla \cdot (\lambda \nabla \vartheta) + \rho \mathbf{f} \cdot \mathbf{u} - \sum_{j=1}^4 h_j^0 w_j, \\ \partial_t (\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{u}) = w_i + \nabla \cdot (D_i \nabla Y_i), \end{cases} \quad (9)$$

for $i = {}^3\text{He}, {}^4\text{He}, {}^7\text{Be}, n$.

If we further assume that ${}^3\text{He}$ and ${}^7\text{Be}$ are present only by trace amounts in the mixture, and that the ${}^4\text{He}$ and the neutrons are in excess, we can suppose that $Y_{{}^4\text{He}}$ and Y_n are constant and then we write

$$\begin{cases} Y_{{}^4\text{He}} = Y_{{}^4\text{He}}^0, \\ Y_n = Y_n^0, \\ Y_{{}^3\text{He}} \ll Y_{{}^4\text{He}}^0 + Y_n^0, \\ Y_{{}^7\text{Be}} \ll Y_{{}^4\text{He}}^0 + Y_n^0, \end{cases}$$

and the equations for $Y_{{}^4\text{He}}$ and Y_n are decoupled. The only remaining equation is that corresponding to ${}^3\text{He}$ (with $Z := Y_{{}^3\text{He}}$) and we recover the simplest combustion model for reacting fluids [4]

$$\partial_t \varrho + \nabla \cdot (\varrho \mathbf{u}) = 0, \quad (10)$$

$$\partial_t (\varrho \mathbf{u}) + \text{div}(\varrho \mathbf{u} \otimes \mathbf{u}) + \nabla_x p = \text{div} \mathbb{S} + \varrho \nabla_x \Psi, \quad (11)$$

$$\partial_t (\varrho e) + \text{div}(\varrho e \mathbf{u}) + \text{div} \mathbf{q} = \Phi - p \text{div} \mathbf{u} + h w(\varrho, \vartheta, Z), \quad (12)$$

$$-\Delta \Psi = G \varrho \text{ on } R^3, \quad (13)$$

$$\partial_t (\varrho Z) + \text{div}(\varrho Z \mathbf{u}) = -\text{div} \mathbf{F} + w(\varrho, \vartheta, Z), \quad (14)$$

where the chemical source w is

$$w(Z, T) := -\varrho Z A,$$

where A is the (positive) reaction rate.

From the previous considerations, we have to solve the system (10)-(14) for the density $\varrho = \varrho(t, x)$, the velocity $\mathbf{u} = \mathbf{u}(t, x)$, the absolute temperature $\vartheta = \vartheta(t, x)$, and the concentration Z , evaluated at the time $t \in [0, T]$ and the reference spatial position $x \in \Omega \subset R^3$.

In (13) p is the pressure, \mathbb{S} stands for the viscous stress tensor, and $\nabla_x \Psi$ is the extraneous force acting on the mixture due to self-gravitation, where the potential Ψ solves the *Poisson equation* (13) where ϱ is extended to be zero outside Ω .

In (12) \mathbf{q} denotes the heat energy flux, Φ is the *dissipation function* representing the irreversible transfer of the mechanical energy into heat and h is a positive constant.

In (14) \mathbf{F} is the diffusion flux.

If the motion is smooth enough, the momentum equation (11) can be multiplied on \mathbf{u} in order to obtain

$$\begin{aligned} \partial_t \left(\frac{1}{2} \rho |\mathbf{u}|^2 - \frac{G}{2} \Delta^{-1} [\rho] \rho \right) + \operatorname{div} \left(\left(\frac{1}{2} \rho |\mathbf{u}|^2 + p \right) \mathbf{u} \right) \\ = \operatorname{div}(\mathbb{S}\mathbf{u}) + p \operatorname{div} \mathbf{u} - \mathbb{S} : \nabla_x \mathbf{u} + \operatorname{div}(\rho \Psi \mathbf{u}), \end{aligned} \quad (15)$$

where $\frac{1}{2} \rho |\mathbf{u}|^2$ denotes the *kinetic energy*.

The total energy $E \equiv \frac{1}{2} \rho |\mathbf{u}|^2 + \rho e + h \rho Z - \frac{1}{2} \rho G \Delta^{-1} [\rho] \rho + h \rho Z$ being a conserved quantity

$$\frac{d}{dt} \int_{\Omega} E(t) dx = 0, \quad (16)$$

we get

$$\Phi = \mathbb{S} : \nabla_x \mathbf{u} \quad (17)$$

provided the motion characterized by the velocity \mathbf{u} is smooth. In general, one can assert only

$$\Phi \geq \mathbb{S} : \nabla_x \mathbf{u}. \quad (18)$$

Finally, assuming that $p = p(\rho, \vartheta)$ and $e = e(\rho, \vartheta)$ are explicit functions of the density, the absolute temperature, we get the specific entropy through the thermodynamical relationship:

$$\frac{\partial s}{\partial \rho} = \frac{1}{\vartheta} \left(\frac{\partial e}{\partial \rho} - \frac{p}{\rho^2} \right), \quad \frac{\partial s}{\partial \vartheta} = \frac{1}{\vartheta} \frac{\partial e}{\partial \vartheta}, \quad (19)$$

Accordingly, the internal energy balance (12) may be put into an equivalent form of the entropy equation

$$\partial_t(\rho s) + \operatorname{div}(\rho s \mathbf{u}) + \operatorname{div} \left(\frac{\mathbf{q}}{\vartheta} \right) = \frac{\Phi}{\vartheta} - \frac{\mathbf{q} \cdot \nabla_x \vartheta}{\vartheta^2} + h \frac{w}{\vartheta}. \quad (20)$$

By virtue of the Clausius-Duhem inequality, the right-hand side of (20) must be non-negative for any possible motion, so

$$\Phi \geq \mathbb{S} : \nabla_x \mathbf{u} \geq 0, \quad \mathbf{q} \cdot \nabla_x \vartheta \leq 0. \quad (21)$$

We suppose that the state variables ρ and ϑ , including the radiation (taking into account the photons γ in (7)), is provided by the general form:

$$p = p_G + p_R,$$

with a gaseous contribution

$$p_G = p_e(\rho) + \vartheta p_\vartheta(\rho), \quad (22)$$

where the elastic pressure p_e as well as the thermal pressure component p_ϑ are continuously differentiable functions of the density, and we assume that

$$p_e(0) = 0, \quad p'_e(\rho) \geq a_1 \rho^{\gamma-1} - c_1, \quad p_e(\rho) \leq a_2 \rho^\gamma + c_2, \quad (23)$$

$$p_\vartheta(0) = 0, \quad p'_\vartheta(\rho) \geq 0, \quad p_\vartheta(\rho) \leq a_3 \rho^\Gamma + c_3, \quad (24)$$

with

$$a_1 > 0, \quad \gamma \geq 2, \quad \gamma > \frac{4\Gamma}{3}. \quad (25)$$

The radiative pressure term has the form

$$p_R = \frac{d}{3}\vartheta^4, \quad (26)$$

where $d > 0$ is the Stefan-Boltzmann constant. Consequently, we have

$$p = p(\varrho, \vartheta) = p_G(\varrho, \vartheta) + p_R(\varrho, \vartheta) = p_e(\varrho) + \vartheta p_\vartheta(\varrho) + \frac{d}{3}\vartheta^4. \quad (27)$$

According (19), the corresponding form of the internal energy density reads

$$e(\varrho, \vartheta) = P_e(\varrho) + d\frac{\vartheta^4}{\varrho} + Q(\vartheta), \quad (28)$$

where Q is a non-decreasing function of the temperature. More specifically, the quantity

$$c_v(\vartheta) = Q'(\vartheta)$$

is termed the specific heat at constant volume.

For the sake of simplicity, we shall assume c_v to be a positive constant, which yields

$$s(\varrho, \vartheta) = \frac{4}{3}d\frac{\vartheta^3}{\varrho} - P_\vartheta(\varrho) + c_v \log(\vartheta), \quad (29)$$

where

$$P_e(\varrho) = \int_1^\varrho \frac{p_e(z)}{z^2} dz, \quad P_\vartheta(\varrho) = \int_1^\varrho \frac{p_\vartheta(z)}{z^2} dz. \quad (30)$$

We restrict now the study to Newtonian fluids for which the viscosity tensor \mathbb{S} is a linear function of the velocity gradient,

$$\mathbb{S} = \mu(\nabla_x \mathbf{u} + {}^t \nabla_x \mathbf{u}) + \lambda \operatorname{div} \mathbf{u} \mathbb{I}, \quad (31)$$

with the shear viscosity coefficient μ , and the bulk viscosity coefficient $\zeta = \lambda + \frac{2}{3}\mu$. After (21), both μ and ζ must be non-negative.

The heat flux \mathbf{q} will be taken through the classical Fourier law:

$$\mathbf{q} = -\kappa \nabla_x \vartheta, \quad (32)$$

with the heat conductivity coefficient κ .

For the diffusion flux \mathbf{F} , we follow the Fick's law

$$\mathbf{F} = -\varrho d \kappa \nabla_x Z a, \quad (33)$$

with the diffusion coefficient d .

As generally, both viscosity and heat conductivity of a gas depend on the temperature, we suppose that

$$\left\{ \begin{array}{l} 0 < \underline{\mu}(1 + \vartheta^\beta) \leq \mu(\vartheta), \quad |\mu'(\vartheta)| \leq \overline{\mu}(1 + \vartheta)^{\beta-1}, \\ \zeta \geq 0, \quad \underline{\zeta} \vartheta^\beta - 1 \leq \zeta(\vartheta), \quad |\zeta'(\vartheta)| \leq \overline{\zeta}(1 + \vartheta)^{\beta-1}. \end{array} \right\} \quad (34)$$

Similarly, we set

$$\kappa = \kappa_G(\vartheta) + \kappa_R(\varrho, \vartheta), \quad (35)$$

with

$$0 < \underline{\kappa}_G \leq \kappa_G(\vartheta) \leq \overline{\kappa}_G(1 + \vartheta^\alpha), \quad (36)$$

and the *radiative term*

$$\underline{\kappa}\vartheta^\alpha \leq \kappa_R(\varrho, \vartheta) \leq \overline{\kappa}(1 + \vartheta^\alpha). \quad (37)$$

As a matter of fact, the quantity σ itself depends on ϱ and ϑ in a rather complicated way. For the sake of simplicity, however, we consider the “zero order” approximation taking σ a positive constant).

Finally, the flux diffusion coefficient $D = \varrho d$ is supposed to be a continuously differentiable function depending on the temperature, such that

$$0 \leq \underline{D}(\vartheta) \leq \overline{D}(1 + \vartheta^\beta), \quad \text{for all } \vartheta > 0, \quad (38)$$

with positive coefficients \underline{D} and \overline{D} , and the reaction rate is also supposed to be a continuously differentiable function depending on the temperature, such that

$$0 \leq A(\vartheta) \leq \overline{A}\vartheta, \quad \text{for all } \vartheta > 0, \quad (39)$$

with positive coefficient \overline{A} .

In order to obtain, at least formally, a well-posed problem, we take a no-slip boundary condition for the velocity field:

$$\mathbf{u}|_{\partial\Omega} = 0, \quad (40)$$

a thermally isolate condition for the temperature

$$\mathbf{q} \cdot \mathbf{n}|_{\partial\Omega} = 0, \quad (41)$$

where \mathbf{n} denotes the outer normal vector, and a no-diffusion condition for the diffusion flux

$$\mathbf{F} \cdot \mathbf{n}|_{\partial\Omega} = 0, \quad (42)$$

However, it is not known if, given the initial state variables:

$$\varrho(0, \cdot) = \varrho_0, \quad \varrho \mathbf{u}(0, \cdot) = \mathbf{m}_0, \quad \vartheta(0, \cdot) = \vartheta_0, \quad Z(0, \cdot) = Z_0, \quad (43)$$

a classical (smooth) solution of the problem satisfying the initial conditions (43) exists on an arbitrarily large time interval $(0, T)$.

In order to avoid this difficulty, it is shown in [28] how to develop a mathematical theory based on the concept of variational solutions (recall that the first rigorous results for compressible fluids were presented by P.-L. Lions [43] and see also [23] for the astrophysical non-reactive context).

In the present reactive case, we say that the functions

$$\varrho \in L^\infty(0, T; L^\gamma(\Omega)), \quad \mathbf{u} \in L^2(0, T; W_0^{1,2}(\Omega; \mathbb{R}^3)), \quad \vartheta \in L^2(0, T; W^{1,2}(\Omega)),$$

and

$$Z \in L^\infty((0, T); \Omega) \cap L^2(0, T; W^{1,2}(\Omega)),$$

represent a variational solution of the problem (10)-(14), (16), (43), if

1. the density ϱ is non-negative on $(0, T) \times \Omega$,

$$\log \vartheta \in L^2(0, T; W^{1,2}(\Omega)),$$

and

$$0 \leq Z(t, x) \leq 1 \quad \text{for a.a. } (t, x) \in (0, T) \times \Omega.$$

2. the continuity equation (10) is satisfied in the distribution sense $\mathcal{D}'(0, T \times \mathbb{R}^3)$, provided that ϱ, \mathbf{u} are zero outside Ω .
3. the dynamical equation (11) holds in $\mathcal{D}'((0, T) \times \Omega)$ and the gravitational potential Φ is obtained from the Poisson equation (13) considered on \mathbb{R}^3 ,
4. the specific entropy s satisfies the inequality

$$\int_0^T \int_{\Omega} \varrho s \partial_t \varphi + \varrho \mathbf{s} \mathbf{u} \cdot \nabla_x \varphi + \frac{\mathbf{q}}{\vartheta} \cdot \nabla_x \varphi \, dx \, dt \leq \tag{44}$$

$$\int_0^T \int_{\Omega} \left(\frac{\mathbf{q} \cdot \nabla_x \vartheta}{\vartheta^2} - \frac{\mathbb{S} : \nabla_x \mathbf{u}}{\vartheta} \right) \varphi + \frac{h \varrho Z A}{\vartheta} \, dx \, dt$$

for any non-negative function $\varphi \in \mathcal{D}((0, T) \times \overline{\Omega})$,

5. the reactant fraction Z satisfies the identity

$$\int_0^T \int_{\Omega} \varrho Z \partial_t \varphi + \varrho Z \mathbf{u} \cdot \nabla_x \varphi - \varrho d \nabla_x Z \cdot \nabla_x \varphi \, dx \, dt = \tag{45}$$

$$\int_0^T \int_{\Omega} \varrho Z A \varphi \, dx \, dt$$

for any function $\varphi \in \mathcal{D}((0, T) \times \overline{\Omega})$,

6. the total energy E is a constant of motion:

$$\int_{\Omega} E(t_1) \, dx = \int_{\Omega} E(t_2) \, dx, \quad \text{for any Lebesgue points } t_1, t_2 \in (0, T).$$

One can check that for any variational solution of the previous problem, the internal energy equation

$$\partial_t(\varrho e) + \operatorname{div}(\varrho e \mathbf{u}) + \operatorname{div} \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{u} - p \operatorname{div} \mathbf{u} + h \varrho Z A$$

holds in $(0, T) \times \overline{\Omega}$.

Under the previous conditions, the following result due to E. Feireisl and A. Novotny [29] holds (see also D. Donatelli and K. Trivisa [16] for different hypotheses),

THEOREM 1. *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with a boundary of class $C^{2+\nu}$, $\nu > 0$. Suppose that the pressure p is determined through the state equation (27), with $d > 0$, and p_e, p_{ϑ} satisfying (23 - 25). Furthermore, let the viscous stress tensor \mathbb{S} be given by (31), where μ and ζ are continuous differentiable globally Lipschitz functions of ϑ obeying (34) for $0 \leq \alpha \leq \frac{4}{3}$.*

Let \mathbf{q} be given by (32) with κ satisfying (35 - 37) for $\alpha \geq \frac{16}{3} - \beta$, and similarly, let $D = \varrho d$ be given by (38) and the reaction rate A be given by (39).

Finally, assume the initial data $\varrho_0, \mathbf{u}_0, \vartheta_0, Z_0$ satisfy

$$\left\{ \begin{array}{l} \varrho_0, \vartheta_0, Z_0 \in L^{\infty}(\Omega), \mathbf{u}_0 \in L^{\infty}(\Omega; \mathbb{R}^3), \\ \vartheta_0 \geq 0, \quad 0 < \underline{\vartheta} \leq \vartheta(x) \leq \overline{\vartheta}, \\ 0 \leq Z(x) \leq 1, \quad \text{for a.a. } x \in \Omega. \end{array} \right\} \tag{46}$$

Then for any given $T > 0$, the problem (10)-(14), (16), (43), (40), (41), (42) possesses a variational solution on the set $(0, T) \times \Omega$ in the sense of the previous definition, moreover

this solution satisfies the initial conditions

$$\left\{ \begin{array}{l} \varrho(t) \rightarrow \varrho_0, \text{ in } L^1(\Omega), \\ (\varrho Z)(t) \rightarrow \varrho_0 Z_0 \text{ weakly in } L^1(\Omega), \end{array} \right\} \quad (47)$$

as $t \rightarrow 0+$, moreover

$$\text{ess } \lim_{t \rightarrow 0+} \int_{\Omega} (\varrho s)(t) \phi \, dx \geq \int_{\Omega} \varrho_0 s_0 \phi \, dx, \quad (48)$$

for any $\phi \geq 0$, $\phi \in \mathcal{D}'(\Omega)$, where

$$\varrho_0 s_0 = \frac{4d}{3} \vartheta_0^3 - \varrho_0 P_{\vartheta}(\varrho_0) + c_v \varrho_0 \log(\vartheta_0).$$

4. A one-dimensional model. Our purpose in this section is to consider a simplified model of multicomponent fluid with a unique chemical reaction, in the framework of 1D-flows.

We suppose that the species E_1, \dots, E_N interact through the chemical reaction

$$\sum_{i=1}^N \alpha_i E_i \rightarrow \sum_{i=1}^N \beta_i E_i, \quad (49)$$

where α_i, β_i are the stoichiometric coefficients of species i in the chemical reaction.

The problem under study is then the following compressible Navier–Stokes system in the lagrangian setting [1] describing 1D-flows of a viscous heat-conducting radiative and reactive gas for a N species mixture

$$\eta_t = v_x, \quad (50)$$

$$v_t = \sigma_x, \quad (51)$$

$$e_t = q_x + \sigma v_x, \quad (52)$$

$$(Y_i)_t = (J_i)_x + \omega_i, \quad i = 1, \dots, N, \quad (53)$$

for $(x, t) \in Q \equiv \Omega \times \mathbf{R}^+ = (0, M) \times (0, \infty)$, where x, t are the Lagrangian mass coordinates.

The first equations (50)-(52) describe the flow of the mixture (specific volume η , velocity v , temperature θ) and the set of equations (53) for $i = 1, \dots, N$ is a reaction-diffusion system describing the concentrations Y_i of the individual species.

We choose the state functions p (pressure), e (specific internal energy) and s (specific entropy) of the form

$$p(\eta, \theta, \{Y_i\}_{i=1, \dots, N}) = \sum_{i=1}^N \frac{R_i Y_i \theta}{\eta} + \frac{a}{3} \theta^4, \quad (54)$$

and

$$e(\eta, \theta, \{Y_i\}_{i=1, \dots, N}) = \sum_{i=1}^N c_{V_i} Y_i \theta + a \eta \theta^4. \quad (55)$$

$$s(\eta, \theta, \{Y_i\}_{i=1, \dots, N}) = \sum_{i=1}^N (R_i \log \eta_i + c_{V_i} \log \theta) + \frac{4}{3} a \eta \theta^3, \quad (56)$$

with $\eta_i = \frac{1}{\rho_i}$ and $\rho_i = \rho Y_i$.

This choice corresponds to a mixture of perfect gases with a radiating part (photon gas) in local thermodynamical equilibrium.

For the stress we take a linearly viscous model for the mixture

$$\sigma(\eta, \theta, \{Y_i\}_{i=1, \dots, N}) = -p(\eta, \theta, \{Y_i\}_{i=1, \dots, N}) + \nu \rho v_x, \quad (57)$$

where $\rho = \frac{1}{\eta}$.

The heat flux is

$$q = -\kappa \rho \theta_x + \sum_{i=1}^N \rho Y_i V_i h_i, \quad (58)$$

where the diffusion velocities follow the simple Fick's law

$$V_i = -D_i \frac{(Y_i)_x}{Y_i}, \quad (59)$$

with the individual enthalpy $h_i = c_{P_i} \theta$.

We adopt a simple form for the diffusion flux (see LANDAU [40] for more general models and [49] for a mathematical analysis of these models)

$$J_i = \rho Y_i V_i. \quad (60)$$

The molar production rates ω_i for $i = 1, \dots, N$ are given functions of the form

$$\begin{aligned} \omega_i(\{\alpha_j, \beta_j\}_{j=1, \dots, N}; \eta, \theta, \{Y_j\}_{j=1, \dots, N}) \\ = A_i \theta^{a_i} e^{-\frac{e_i}{r\theta}} \rho^b \tilde{\omega}_i(\{\alpha_j, \beta_j\}_{j=1, \dots, N}; \{Y_j\}_{j=1, \dots, N}) \end{aligned} \quad (61)$$

where the coefficients A_i, a_i, e_i, r, b are positive and the functions $\tilde{\omega}_i$ depending on the Y_i and the stoichiometric coefficients α_i, β_i , may be negative (destruction of species i) or positive (production of species i).

More precisely we assume that

$$\tilde{\omega}_i(\{\alpha_j, \beta_j\}_{j=1, \dots, N-1}; \{Y_j\}_{j=1, \dots, N-1}) \leq 0, \quad \text{for } 1 \leq i \leq N-1. \quad (62)$$

Moreover we suppose that the ω_i satisfy the global mass conservation

$$\sum_{i=1}^N \omega_i = 0, \quad (63)$$

Finally, it will be useful to consider the evolution equation for the balance of entropy

$$s_t + (j_S)_x = \varsigma_S, \quad (64)$$

where the entropy flux j_S is

$$j_S = \frac{1}{\theta} \left(q - \sum_{i=1}^N \rho Y_i V_i \mu_i \right), \quad (65)$$

the entropy source is

$$\varsigma_S = -\frac{1}{\theta^2} q \theta_x - \sum_{i=1}^N \rho Y_i V_i \left(\frac{\mu_i}{\theta} \right)_x + \frac{1}{\theta} \nu \rho v_x^2 - \frac{1}{\theta} \sum_{i=1}^N \mu_i \omega_i, \quad (66)$$

where the chemical potential μ_i is computed using the thermodynamical Gibbs relation

$$\theta ds = de + pd\left(\frac{1}{\rho}\right) - \sum_{i=1}^N \mu_i Y_i.$$

For the perfect gas i , the chemical potential μ_i is [5]

$$\mu_i(\eta, \theta, Y_i) = \mu_i^0 + \log \frac{p_i}{p_0}, \tag{67}$$

with $p_i(\eta, \theta) = \frac{R_i Y_i \theta}{\eta}$, for an arbitrary reference state (μ_i^0, p_0) .

We take the following boundary conditions

$$v|_{x=0} = 0, \quad \sigma|_{x=M} = -p_\Gamma, \tag{68}$$

$$q|_{x=0} = 0, \quad \theta|_{x=M} = \theta_\Gamma, \tag{69}$$

$$J_i|_{x=0, M} = 0, \quad \text{for } i = 1, \dots, N - 1. \tag{70}$$

with given $p_\Gamma = \text{const} > 0$ and $\theta_\Gamma = \text{const} > 0$, together with the initial conditions

$$(\eta, v, \theta, Y_i)|_{t=0} = (\eta^0(x), v^0(x), \theta^0(x), Y_i^0(x)), \quad \text{for } x \in \Omega, \quad i = 1, \dots, N. \tag{71}$$

The unknown quantities $\eta > 0$, $v, \theta > 0$ and $0 \leq Y_i \leq 1$ are the specific volume, the velocity, the absolute temperature and the concentration of species i , with the mass constraint

$$\sum_{i=1}^N Y_i = 1. \tag{72}$$

Finally $\kappa(\eta, \theta)$, p_Γ and θ_Γ are the heat conductivity, the outer pressure and the outer temperature, and the quantities $\nu, R_i, a, c_{V_i}, c_{P_i}, D_i, \nu$ and d are positive physical constants as well as M is the total mass of the gas.

In the simple case of section 3, for arbitrarily large data, it is possible to prove [26] (see also the references therein and [3] [4] [8] [12] [13] [14] [19] [20] [35] [52] for related works on this model) global (in time) bounds for the solution of the above problem and establish its global exponential decay as $t \rightarrow \infty$ in suitable spaces.

We show in the following that the Lyapunov functional method may be partially extended to the multicomponent case.

4.1. Statement of the results. In the following, we use the classical Lebesgue and Sobolev spaces $L^q(G)$ and $W^{1,q}(G)$, for $q \in [1, \infty]$, with $H^1(G) = W^{1,2}(G)$ and $H^0(G) = L^2(G)$. We also need the anisotropic Lebesgue and Sobolev spaces $L^{q,r}(Q_T)$ and $H^{2,1}(Q_T) \equiv W_2^{2,1}(Q_T)$, for $Q_T := \Omega \times (0, T)$ with $0 < T \leq \infty$ (see [41]), with the norms

$$\begin{aligned} \|w\|_{L^{q,r}(Q_T)} &= \left\| \|w\|_{L^q(\Omega)} \right\|_{L^r(0,T)}, \\ \|w\|_{H^{2,1}(Q_T)} &= \|w\|_{V_2(Q_T)} + \|w_x\|_{V_2(Q_T)} + \|w_t\|_{L^2(Q_T)}, \end{aligned}$$

where $V_2(Q_T)$ is the standard space of functions w on Q_T having finite (parabolic) energy $\|w\|_{V_2(Q_T)} = \|w\|_{L^{2,\infty}(Q_T)} + \|w_x\|_{L^2(Q_T)}$. We define the following integration operators, for $(x, t) \in \bar{Q}$

$$(I\varphi)(x) = \int_0^x \varphi(\xi) d\xi, \quad (I^*\varphi)(x) = \int_x^M \varphi(\xi) d\xi, \quad (I_0y)(t) = \int_0^t y(\tau) d\tau$$

and denote by $\langle \varphi \rangle = \frac{1}{M} \int_{\Omega} \varphi(x) dx$ the mean value over Ω , for any $\varphi \in L^1(\Omega)$.

We assume that $\kappa(\eta, \theta)$ is strictly positive and continuously differentiable on $\mathbf{R}^+ \times \overline{\mathbf{R}}^+$, moreover we suppose that

$$\kappa_1\eta + \kappa_2 \leq \kappa(\eta, \theta),$$

where $\kappa_1 > 0$ and $\kappa_2 > 0$.

We limit ourselves to the case of global solution with strong components (η, v, θ) such that

$$\eta, \eta_x, \eta_t \in L^{2,\infty}(Q_T), \quad \min_{\overline{Q_T}} \eta > 0; \quad v, \theta \in H^{2,1}(Q_T), \quad \theta > 0 \text{ in } \overline{\Omega} \times (0, T], \quad (73)$$

and $Y_i \in V_2(Q_T)$, for any $i = 1, \dots, N$ and any $T < \infty$. The following requirements on the data are necessary

$$\eta^0, v^0, \theta^0 \in H^1(\Omega), \quad \min_{\overline{\Omega}} \eta^0 > 0, \quad \theta^0 \geq 0, \quad v^0(0) = 0, \quad \theta^0(M) = \theta_{\Gamma}. \quad (74)$$

We also suppose that $Y_i^0 \in L^\infty(\Omega)$, for any $i = 1, \dots, N$.

Let us start with the stationary problem, defined by the system

$$\begin{cases} v_x = 0, \\ q_x = 0, \\ (J_i)_x + \omega_i = 0, \quad i = 1, \dots, N, \end{cases} \quad (75)$$

together with (57), for $x \in \Omega$, and also with the first relation (54), under the boundary conditions (68)–(70).

PROPOSITION 1. *Suppose that the chemical sources ω_i satisfy the additional condition “The algebraic system*

$$\tilde{\omega}_i(\{\alpha_j, \beta_j\}_{j=1, \dots, N-1}; \{Y_j\}_{j=1, \dots, N-1}) = 0, \quad i = 1, \dots, N-1, \quad (76)$$

has a unique solution $(y_1, \dots, y_{N-1}) \in \mathbf{R}^{N-1}$, with $0 \leq y_i \leq 1$, for $i = 1, \dots, N-1$.”

Suppose also that the condition

$$\frac{a}{3}\theta_{\Gamma}^4 < p_{\Gamma}, \quad (77)$$

is valid.

Then, the weak solution $\eta_S, v_S, \theta_S, Y_{iS}$, $i = 1, \dots, N$ in $W^{1,1}(\Omega)$ of the stationary problem satisfying $\min_{\overline{\Omega}} \eta_S > 0$ and $\theta_S \geq 0$ exists, and under conditions (76) and (77), the solution is such that

$$\begin{cases} Y_{iS}(x) \equiv y_i, \quad i = 1, \dots, N, \\ v_S(x) \equiv 0, \\ \theta_S(x) \equiv \theta_{\Gamma}, \\ \rho_S(x) \equiv \frac{p_{\Gamma} - \frac{a}{3}\theta_{\Gamma}^4}{\sum_{i=1}^N R_i y_i \theta_{\Gamma}}, \end{cases} \quad (78)$$

with $\rho_S = \frac{1}{\eta_S}$ and $y_N = 1 - \sum_{i=1}^{N-1} y_i$.

Proof. As $\omega_i \leq 0$ for $i = 1, \dots, N - 1$, multiplying the last equation (75) by Y_i and integrating by parts on Ω , we find

$$\int_{\Omega} \rho_S(x) D_i \overline{Y_{iS}^2}(x) dx \leq 0,$$

for $i = 1, \dots, N - 1$, which implies that $Y_{iS} = \text{const}_i = y_i$ for $i = 1, \dots, N$, using (76).

By the second equation (75) and the boundary condition: $q_S = \text{const} = 0$ which implies $\theta_S(x) \equiv \theta_{\Gamma}$.

As the velocity v_S is clearly zero by the boundary condition, the equation for the stress reads

$$p(\eta_S, v_S, \theta_S, \{Y_{iS}\}) = \sum_{i=1}^N R_i y_i \rho_S(x) \theta_{\Gamma} + \frac{a}{3} \theta_{\Gamma}^4 = p_{\Gamma},$$

which gives ρ_S , provided (77) is satisfied. ■

Let $\mathcal{N} > 1$ be an arbitrarily large parameter and $K = K(\mathcal{N})$, $K_i = K_i(\mathcal{N})$, $i = 0, 1, \dots$, be positive nondecreasing functions of \mathcal{N} which can depend also on the physical constants of the problem, and also on $\underline{\eta}$ from (82) below but not directly on the initial data.

Let $\Psi(\zeta) := \zeta - \log \zeta - 1$, for $\zeta > 0$.

THEOREM 1. *Suppose that the data are such that*

$$\mathcal{N}^{-1} \leq \eta^0 \leq \mathcal{N}, \quad \|v^0\|_{L^2(\Omega)} + \|\theta^0\|_{L^4(\Omega)} + \|\log \theta^0\|_{L^1(\Omega)} \leq \mathcal{N}, \tag{79}$$

$$0 \leq Y_i^0 \leq 1, \tag{80}$$

$$(1 + \mathcal{N}^{-1}) \frac{a}{3} \theta_{\Gamma}^4 \leq p_{\Gamma}. \tag{81}$$

Then:

1. *The following bounds in Q hold*

$$0 < \underline{\eta} \leq \eta(x, t) \leq \overline{\eta} = K \quad \text{in } \overline{Q}, \tag{82}$$

$$\|\eta - \eta_S\|_{L^2(Q)} + \|v\|_{V_2(Q)} + \|\frac{v_x}{\sqrt{\theta}}\|_{L^2(Q)} + \|\sigma + p_{\Gamma}\|_{L^2(Q)} \leq K, \tag{83}$$

$$\|\theta\|_{L^{4,\infty}(Q)} + \|\log \theta\|_{L^{1,\infty}(Q)} + \|\frac{\sqrt{K}}{\theta} \theta_x\|_{L^2(Q)} \leq K, \tag{84}$$

$$0 \leq Y_i(x, t) \leq 1 \quad \text{in } \overline{Q}, \tag{85}$$

$$\|\omega_i(\rho, \theta, \{Y_j\}_{j=1,\dots,N})\|_{L^1(Q)} \leq \mathcal{N}, \quad \|Y_{ix}\|_{L^2(Q)} \leq K. \tag{86}$$

2. *The following stabilization properties of the solution hold*

$$\begin{aligned} \mathbf{V}^{(1)}(t) &:= \int_{\Omega} [(\eta(x, t) - \eta_S(x))^2 + v^2(x, t) \\ &+ (1 + \theta(x, t))^2 (\theta(x, t) - \theta_{\Gamma})^2 + \Psi(\frac{\theta(x, t)}{\theta_{\Gamma}})] dx \rightarrow 0, \end{aligned} \tag{87}$$

$$\|Y_i(\cdot, t) - Y_{iS}\|_{L^2(\Omega)} \rightarrow 0, \tag{88}$$

as $t \rightarrow \infty$.

For completeness, let us state the corresponding global existence and uniqueness result.

THEOREM 2. *Under the hypotheses of Theorem 1 (recall that conditions (74) and $Y_i^0 \in L^\infty(\Omega)$ are supposed there), there exists a unique global solution to the problem (50)–(71) satisfying properties (73) along with $Y_i \in V_2(Q_T)$.*

The proof may be adapted from [26]: we start from a local existence result, using our recent approach from [25] based mainly on the theory of $V_2(Q_T)$ and $H^{2,1}(Q_T)$ solutions of linear parabolic problems. The local solution appears simply as a fixed point of a specific nonlinear operator due to the Schauder fixed point theorem. Finally we use the previous a-priori estimates to get a global solution.

4.2. Sketch of the proof of Theorem 1. The proof mainly follows the strategy developed in [26] and relies on the behaviour of suitable Lyapunov functionals [22].

Let $\|\cdot\|_G = \|\cdot\|_{L^2(G)}$ and $z_+ = \max\{z, 0\}$ for brevity. We shall use sometimes another notation for the compositions $b[\eta, \theta](x, t) = b(\eta(x, t), \theta(x, t))$, for $b = e, p, \kappa$, etc.

Suppose that the hypotheses of Theorem 1 are valid. By the definition and the conservation property (72) of species, one knows first that

$$0 \leq Y_i(x, t) \leq 1 \text{ in } Q.$$

LEMMA 1. *The following equality holds*

$$\frac{d}{dt} \langle Y_i \rangle + \langle \omega_i \rangle = 0 \text{ for } i = 1, \dots, N - 1, \text{ on } \mathbf{R}^+. \tag{89}$$

Consequently the following bound in Q and properties of the function $\langle Y_i \rangle$ hold

$$|\int_Q \omega_i \, dx \, dt| = \|\int_\Omega \omega_i \, dx\|_{L^1(\mathbf{R}^+)} \leq 2M, \tag{90}$$

$$\langle Y_i(\cdot, t) \rangle \geq 0 \text{ is nonincreasing for } 0 \leq i \leq N - 1, \text{ for } t \geq 0,$$

$$\langle Y_N(\cdot, t) \rangle \geq 0 \text{ is nondecreasing, for } t \geq 0,$$

$$\langle Y_i(\cdot, t) \rangle \rightarrow Y_{iS} \text{ for } i = 1, \dots, N, \text{ as } t \rightarrow \infty, \tag{91}$$

for some $0 \leq Y_{iS} \leq 1$.

Proof. Equality (89) follows from (53) and (70).

Using $Y_i|_{t=0} = Y_i^0$, one gets

$$\langle Y_i \rangle + \int_0^t \langle \omega_i(s) \rangle \, ds = \langle Y_i^0 \rangle,$$

which implies bound (90) and all the properties of $\langle Y_i \rangle$, observing that $\frac{d}{dt} \langle Y_i \rangle \in L^1(0, T)$, for any $T < \infty$ and any $i = 1, \dots, N$. ■

LEMMA 2.

$$\forall i \in (1, N) : \frac{1}{2} \|Y_i\|_\Omega^2 + \int_0^T \int_\Omega \rho^2 D_i Y_{ix}^2 \, dx \leq K. \tag{92}$$

Proof. For any $i \leq N - 1$, multiplying (53) by Y_i , integrating by parts and using boundary conditions (70) and condition (62), we have

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \sum_{i=1}^N Y_i^2 dx + \int_{\Omega} \sum_{i=1}^N \rho^2 D_i Y_{ix}^2 dx \leq 0,$$

which gives (92) after integrating on $(0, T)$. ■

Let us introduce the normalized specific volume and temperature $\tilde{\eta} := \frac{\eta}{\eta_0}$, $\tilde{\theta} := \frac{\theta}{\theta_{\Gamma}}$, where η_0 is a positive constant to be chosen latter, and let us denote by Ψ_r the elementary function $\Psi_r(\zeta) := \zeta^4 - \frac{4}{3}\zeta^3 + \frac{1}{3} \geq 0$.

LEMMA 3. *The following inequality holds*

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} \left[\theta_{\Gamma} \left(\sum_{i=1}^N R_i \right) \Psi(\tilde{\eta}) + \frac{1}{2} v^2 + \left(\sum_{i=1}^N c_{V_i} \right) \theta_{\Gamma} \Psi(\tilde{\theta}) + \theta_{\Gamma} \sum_{i=1}^N R_i \Psi(Y_i) + a \eta \theta_{\Gamma}^4 \Phi(\tilde{\theta}) \right] dx \\ & \quad + \theta_{\Gamma} \int_{\Omega} \left(\frac{\nu \rho}{\theta} v_x^2 + \frac{\kappa \rho}{\theta^2} \theta_x^2 \right) dx \\ & = \frac{d}{dt} \left(\theta_{\Gamma} \int_{\Omega} \sum_{i=1}^N [R_i Y_i + \mathcal{R} Y_i (\log(R_i Y_i) - 1)] dx \right) + \theta_{\Gamma} \int_{\Omega} \frac{\theta_x}{\theta^2} \sum_{i=1}^N \rho_i V_i h_i dx. \end{aligned} \quad (93)$$

Consequently the following bounds in Q hold

$$\begin{aligned} & \|\Psi(\tilde{\eta})\|_{L^1, \infty(Q)} + \|v\|_{L^2, \infty(Q)} + \|\Psi(\tilde{\theta}) + \eta \Phi(\tilde{\theta})\|_{L^1, \infty(Q)} \\ & \quad + \sum_{i=1}^N \|Y_i\|_{L^2, \infty(Q)} + \sum_{i=1}^N \|Y_i \Psi(Y_i)\|_{L^1, \infty(Q)} \leq K, \end{aligned} \quad (94)$$

$$\left\| \sqrt{\frac{\rho}{\theta}} v_x \right\|_{L^2(Q)} + \left\| \frac{\sqrt{\kappa \rho}}{\theta} \theta_x \right\|_{L^2(Q)} + \sum_{i=1}^N \|\rho \sqrt{D_i} Y_{ix}\|_{L^2(Q)} \leq K. \quad (95)$$

Proof. From (51), (52) one gets

$$\left(\frac{1}{2} v^2 + e \right)_t = (\tau v - q)_x,$$

and using (64)

$$\left(\frac{1}{2} v^2 + e - \theta_{\Gamma} s \right)_t = \left[\tau v - \left(1 - \frac{\theta_{\Gamma}}{\theta} \right) q - \frac{\theta_{\Gamma}}{\theta} \sum_{i=1}^N \rho_i V_i \mu_i \right]_x - \theta_{\Gamma} \varsigma_S.$$

Integrating on Ω and using boundary conditions

$$\frac{d}{dt} \int_{\Omega} \left(P_{\Gamma} \eta + \frac{1}{2} v^2 + e - \theta_{\Gamma} s \right) dx + \theta_{\Gamma} \int_{\Omega} \varsigma_S dx = 0.$$

Using the expression of ς_S , we get

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} \left(p_{\Gamma} \eta + \frac{1}{2} v^2 + e - \theta_{\Gamma} s \right) dx + \theta_{\Gamma} \int_{\Omega} \left(\kappa \rho \frac{\theta_x^2}{\theta^2} + \nu \rho \frac{v_x^2}{\theta} \right) dx \\ & = \theta_{\Gamma} \int_{\Omega} \left(\frac{\theta_x}{\theta^2} \sum_{i=1}^N \rho_i h_i V_i + \sum_{i=1}^N \rho_i V_i \left(\frac{\mu_i}{\theta} \right)_x + \sum_{i=1}^N \frac{\mu_i}{\theta} \omega_i \right) dx. \end{aligned}$$

Using the previously defined renormalized temperature and specific volume, the integrand in the left-hand side reads

$$\mathcal{A} := p_\Gamma \eta + \frac{1}{2} v^2 + e - \theta_\Gamma s = \frac{1}{2} v^2 + \mathcal{A}_1 + \mathcal{A}_2,$$

with

$$\begin{aligned} \mathcal{A}_1 &:= \left(p_\Gamma - \frac{1}{3} a \theta_\Gamma^4 \right) \eta_0 \tilde{\eta} - \theta_\Gamma \left(\sum_{i=1}^N R_i \right) \log \tilde{\eta}, \\ \mathcal{A}_2 &:= -\theta_\Gamma \sum_{i=1}^N R_i \log Y_i + \theta_\Gamma (1 + \log \theta_\Gamma) \sum_{i=1}^N c_{V_i} - \theta_\Gamma \left(\sum_{i=1}^N c_{V_i} \right) \Psi(\tilde{\eta}) + a \eta \theta_\Gamma^4 \Phi(\tilde{\theta}). \end{aligned}$$

Choosing $\eta_0 = \frac{\theta_\Gamma \sum_{i=1}^N R_i}{p_\Gamma - \frac{1}{3} a \theta_\Gamma^4}$, we obtain

$$\mathcal{A}_1 := \theta_\Gamma \left(\sum_{i=1}^N R_i \right) \Psi(\tilde{\eta}) + \theta_\Gamma \left(\sum_{i=1}^N R_i \right).$$

In the same stroke

$$\begin{aligned} \mathcal{A}_2 &:= \theta_\Gamma \sum_{i=1}^N R_i \Psi(Y_i) - \theta_\Gamma \sum_{i=1}^N R_i (Y_i - 1) + \theta_\Gamma (1 + \log \theta_\Gamma) \sum_{i=1}^N c_{V_i} \\ &\quad + \theta_\Gamma \left(\sum_{i=1}^N c_{V_i} \right) \Psi(\tilde{\eta}) + a \eta \theta_\Gamma^4 \Phi(\tilde{\theta}). \end{aligned}$$

So we get

$$\begin{aligned} &\frac{d}{dt} \int_\Omega \left(\theta_\Gamma \left(\sum_{i=1}^N R_i \right) \Psi(\tilde{\eta}) + \frac{1}{2} v^2 + \theta_\Gamma \sum_{i=1}^N R_i \Psi(Y_i) \right. \\ &\quad \left. + \theta_\Gamma \left(\sum_{i=1}^N c_{V_i} \right) \Psi(\tilde{\theta}) + a \eta \theta_\Gamma^4 \Phi(\tilde{\theta}) \right) dx \\ &\quad + \theta_\Gamma \int_\Omega \left(\kappa \frac{\theta_x^2}{\theta^2} + \frac{\nu}{\theta} \rho v_x^2 \right) dx \\ &= \frac{d}{dt} \left(\theta_\Gamma \int_\Omega \sum_{i=1}^N R_i Y_i dx \right) + \theta_\Gamma \int_\Omega \frac{\theta_x}{\theta^2} \sum_{i=1}^N \rho_i h_i V_i dx \\ &\quad + \theta_\Gamma \int_\Omega \left(\sum_{i=1}^N \rho_i V_i \left(\frac{\mu_i}{\theta} \right)_x + \sum_{i=1}^N \frac{\mu_i}{\theta} \omega_i \right) dx := \mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_3. \end{aligned} \tag{96}$$

Integrating by parts in the last term, we have

$$\begin{aligned} \mathcal{B}_3 &= \theta_\Gamma \int_\Omega \left(\sum_{i=1}^N \rho_i V_i \left(\frac{\mu_i}{\theta} \right)_x + \sum_{i=1}^N \frac{\mu_i}{\theta} \omega_i \right) dx \\ &= -\theta_\Gamma \int_\Omega \sum_{i=1}^N D_i \rho^2(Y_i)_x \left(\frac{\mu_i}{\theta} \right)_x dx + \theta_\Gamma \int_\Omega \sum_{i=1}^N \frac{\mu_i}{\theta} \omega_i dx \\ &= \theta_\Gamma \int_\Omega \sum_{i=1}^N (D_i \rho^2(Y_i)_x)_x \frac{\mu_i}{\theta} dx + \theta_\Gamma \int_\Omega \sum_{i=1}^N \frac{\mu_i}{\theta} \omega_i dx = \theta_\Gamma \int_\Omega \sum_{i=1}^N (Y_i)_t \frac{\mu_i}{\theta} dx. \end{aligned}$$

As the chemical potential for perfect gas is $\mu_i = \mu_0 + \mathcal{R}\theta \log \frac{p_i}{p_0}$, where μ_0 and p_0 are reference constants and \mathcal{R} is the perfect gas constant, we compute

$$\frac{\mu_i}{\theta} = \frac{\mu_0}{\theta} + \mathcal{R} \log R_i + \mathcal{R} \log \rho + \mathcal{R} \log \theta + \mathcal{R} \log Y_i + \mathcal{R} \log p_0,$$

using the conservation of species, we conclude that

$$\mathcal{B}_3 = \theta_\Gamma \mathcal{R} \int_\Omega \sum_{i=1}^N (Y_i)_t (\log R_i + \log Y_i) dx.$$

Finally

$$\mathcal{B}_1 + \mathcal{B}_3 = \frac{d}{dt} \left(\theta_\Gamma \int_\Omega \sum_{i=1}^N [R_i Y_i + \mathcal{R} Y_i (\log(R_i Y_i) - 1)] dx \right). \quad (97)$$

Plugging (97) into (96), we get (93).

To get the bounds (94) and (94) we integrate (93) on $(0, T)$, for any $T > 0$

$$\begin{aligned} & \int_\Omega \left[\theta_\Gamma \sum_{i=1}^N R_i \Psi(\tilde{\eta}) + \frac{1}{2} v^2 + \sum_{i=1}^N c_{V_i} \theta_\Gamma \Psi(\tilde{\theta}) + \theta_\Gamma \sum_{i=1}^N R_i \Psi(\tilde{Y}_i) + a\eta \theta_\Gamma^4 \Phi(\tilde{\theta}) \right] dx \\ & \quad + \theta_\Gamma \int_0^T \int_\Omega \left(\frac{\nu \rho}{\theta} v_x^2 + \frac{\kappa \rho}{\theta^2} \theta_x^2 \right) dx dt \\ & = \theta_\Gamma \int_\Omega \sum_{i=1}^N [R_i Y_i + \mathcal{R} Y_i (\log(R_i Y_i) - 1)] dx + \theta_\Gamma \int_0^T \int_\Omega \frac{\theta_x}{\theta} \sum_{i=1}^N \rho_i h_i V_i dx dt \\ & + \int_\Omega \left[\theta_\Gamma \sum_{i=1}^N R_i \Psi(\tilde{\eta}^0) + \frac{1}{2} v^{02} + \sum_{i=1}^N c_{V_i} \theta_\Gamma \Psi(\tilde{\theta}^0) + \theta_\Gamma \sum_{i=1}^N R_i \Psi(\tilde{Y}_i^0) + a\eta^0 \theta_\Gamma^4 \Phi(\tilde{\theta}^0) \right. \\ & \quad \left. - \theta_\Gamma \sum_{i=1}^N [R_i Y_i^0 + \mathcal{R} Y_i^0 (\log(R_i Y_i^0) - 1)] \right] dx. \quad (98) \end{aligned}$$

We can bound \mathcal{B}_2 (the second contribution in (98)) by using the Cauchy-Schwarz inequality and (92)

$$\begin{aligned} |\mathcal{B}_2| & \leq \theta_\Gamma \int_\Omega \frac{|\theta_x|}{\theta} \sum_{i=1}^N R_i D_i c_{P_i} \rho |Y_i| dx \\ & \leq \frac{\epsilon}{2} \theta_\Gamma \int_\Omega \kappa \rho \frac{\theta_x^2}{\theta^2} dx + \frac{1}{2\epsilon} \theta_\Gamma \int_\Omega \frac{\rho}{\kappa} \left(\sum_{i=1}^N R_i D_i c_{P_i} \rho |Y_i| \right)^2 dx \\ & \leq \frac{\epsilon}{2} \theta_\Gamma \int_\Omega \kappa \rho \frac{\theta_x^2}{\theta^2} dx + \frac{\delta}{2\epsilon} \theta_\Gamma \int_\Omega \sum_{i=1}^N D_i \rho^2 (Y_{i,x})^2 dx, \end{aligned}$$

where $\delta = \kappa_1^{-1} \max_i \{R_i^2 D_i c_{P_i}^2\}$, which gives the estimate

$$|\mathcal{B}_2| \leq \frac{\epsilon}{2} \theta_\Gamma \int_\Omega \kappa \rho \frac{\theta_x^2}{\theta^2} dx + K_1(\mathcal{N}), \quad (99)$$

where $\epsilon > 0$.

Finally, using lemma 2 and (98) and for ϵ small enough, we get the inequality

$$\begin{aligned} \int_{\Omega} \left[\theta_{\Gamma} \sum_{i=1}^N R_i \Psi(\tilde{\eta}) + \frac{1}{2} v^2 + \frac{1}{2} \sum_{i=1}^N Y_i^2 + \sum_{i=1}^N c_{V_i} \theta_{\Gamma} \Psi(\tilde{\theta}) + \theta_{\Gamma} \sum_{i=1}^N R_i \Psi(\tilde{Y}_i) + a \eta \theta_{\Gamma}^4 \Phi(\tilde{\theta}) \right] dx \\ + \theta_{\Gamma} \int_0^T \int_{\Omega} \left(\frac{\nu \rho}{\theta} v_x^2 + \frac{\kappa \rho}{\theta^2} \theta_x^2 + \sum_{i=1}^N \rho^2 D_i (Y_{i_x})^2 \right) dx dt \leq K_2(\mathcal{N}), \end{aligned}$$

from which all the estimates (94) and (94) follow. ■

From the previous estimates one gets the following bounds in Q for η and θ

$$\|\eta\|_{L^1, \infty(Q)} \leq K, \quad \|\theta\|_{L^1, \infty(Q)} + \|\log \theta\|_{L^1, \infty(Q)} + \|\eta \theta^4\|_{L^1, \infty(Q)} \leq K. \quad (100)$$

Now, by [26], the following implicit formula for the specific volume η holds

$$\eta = \frac{1}{E(\delta)} \left[\eta^0 + \frac{1}{\nu} I_0(E^{(\delta)} \eta(p - \delta)) \right] \text{ in } \bar{Q}, \quad (101)$$

with a parameter δ , where

$$E^{(\delta)}(x, t) := B(x, t) e^{\frac{1}{\nu} (p_{\Gamma}(x) - \delta)t}, \text{ with } K^{-1} \leq B := e^{\frac{1}{\nu} I^*(v - v^0)} \leq K \text{ in } \bar{Q}.$$

Using this formula together with the energy bounds (100)(104) and (100)(104), we obtain the crucial density bounds

$$0 < \underline{\eta} \leq \eta(x, t) \leq \bar{\eta} \text{ in } \bar{Q}. \quad (102)$$

Then one checks the additional L^p estimates

$$\|\tilde{\theta} - 1\|_{C(\bar{\Omega})} + \|\tilde{\theta}^2 - 1\|_{C(\bar{\Omega})} + \|\sqrt{\tilde{\eta}}(\tilde{\theta}^4 - 1)\|_{L^2(\Omega)} \leq KA, \quad (103)$$

$$\|\Psi(\tilde{\theta})\|_{C(\bar{\Omega})} + \|\eta \Psi_r(\tilde{\theta})\|_{L^1(\Omega)} \leq KA^2, \quad (104)$$

with $A := \|\frac{\sqrt{\rho}}{\theta} \theta_x\|_{L^2(\Omega)}$ satisfying $\|A\|_{L^2(\mathbf{R}^+)} \leq K$.

Using (102), the following inequalities hold for $i = 1, \dots, N$

$$\frac{1}{2} \frac{d}{dt} \|Y_i - \langle Y_i \rangle\|_{\Omega}^2 + D_i \underline{\rho}^2 \|(Y_i)_x\|_{\Omega}^2 \leq \int_{\Omega} Y_i \omega_i dx \text{ on } \mathbf{R}^+. \quad (105)$$

Consequently the second bound (86) follows. Moreover $\frac{d}{dt} \int_{\Omega} (Y_i - \langle Y_i \rangle)^2 dx \in L^1(0, T)$, for any $T < \infty$ and the stabilization property (88) holds.

In the spirit of [26] we introduce now the functionals

$$\begin{aligned} \mathcal{Y}^{(0)} &:= \int_{\Omega} \left\{ \theta_{\Gamma} \left[\left(\sum_{i=1}^N R_i \Psi(\tilde{\eta}_i) \right) + \beta_0 \nu \eta_S \Psi(\tilde{\eta}) \right] + \frac{1}{2} v^2 + \beta_0 \nu I(\eta - \eta_S) \right. \\ &\quad \left. + \theta_{\Gamma} \left(\sum_{i=1}^N c_{V_i} Y_i \right) \Psi(\tilde{\theta}) + a \theta_{\Gamma}^4 \eta \Psi_r(\tilde{\theta}) \right\} dx, \\ \mathcal{Y}^{(0)} &:= \int_{\Omega} \left[\beta_0 \sum_{i=1}^N R_i \rho \rho_S Y_i (\eta - \eta_S)^2 + \frac{\nu}{\theta} \rho v_x^2 - \beta_0 v^2 + \theta_{\Gamma} \frac{\rho \kappa}{\theta^2} \theta_x^2 \right] dx, \\ \mathbf{Y}^{(0)} &:= \int_{\Omega} \left[(\eta - \eta_S)^2 + \frac{v_x^2}{\theta} + \frac{\kappa}{\theta^2} \theta_x^2 \right] dx, \end{aligned}$$

with a parameter β_0 .

Then, reasoning similarly to [26], the following inequality holds

$$\frac{d\mathcal{V}^{(0)}}{dt} + \mathcal{Y}^{(0)} \leq \beta_0 \int_{\Omega} [p(\eta, \theta; \{Y_i\}_{i=1, \dots, N}) - p(\eta, \theta_{\Gamma}; \{Y_{iS}\}_{i=1, \dots, N})] (\eta - \eta_S) dx \quad (106)$$

together with the estimates, for a fixed and sufficiently small $\beta_0 := \frac{1}{K}$,

$$\frac{d\mathcal{V}^{(0)}}{dt} + K^{-1}\mathbf{Y}^{(0)} \leq \int_{\Omega} [p(\eta, \theta; \{Y_i\}_{i=1, \dots, N}) - p(\eta, \theta_{\Gamma}; \{Y_{iS}\}_{i=1, \dots, N})] (\eta - \eta_S) dx \quad (107)$$

$$K^{-1}\mathbf{V}^{(1)} \leq \mathcal{V}^{(0)} \leq K\mathbf{V}^{(1)} \leq K_1\mathbf{Y}^{(0)}, \quad (108)$$

where $\mathbf{V}^{(1)}$ has been introduced in (87).

In fact, due to $\|\theta\|_{L^1(\Omega)} \leq K$ (see (100)), we have

$$\int_{\Omega} v^2 dx \leq M \|v_x\|_{L^1(\Omega)}^2 \leq M \|\theta\|_{L^1(\Omega)} \left\| \frac{v_x}{\sqrt{\theta}} \right\|_{\Omega}^2 \leq MK \left\| \frac{v_x}{\sqrt{\theta}} \right\|_{\Omega}^2.$$

Finally, using the uniform bounds $\underline{\rho} \leq \rho \leq \bar{\rho}$ and choosing $\varepsilon := \frac{1}{K}$ and then $\beta_0 := \frac{1}{K_1}$, both small enough, we obtain (107). Taking into account inequality (104) also, we obtain the last inequality (108) as well. Consequently the stabilization property (87) is valid, which ends the proof of the theorem ■

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