# Fundamental problems to equations
# of compressible chemically reacting flows

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An extended abstract of the PhD dissertation

Multicomponent reactive flows with chemistry and detailed transport phenomena arise in various engineering applications, such as spatial vehicle reentry, crystal growth, combustion and atmospheric pollution [15]. This is a strong motivation for investigating the mathematical structure and properties of the corresponding systems of partial differential equations. In the present thesis we are concerned with the existence theory for the model formulated by the full Navier-Stokes system supplemented by the reaction-diffusion equations for the species. Our principal intention is to handle reversible reactions and the pressure which depends on concentration of the chemical species. As a consequence, one has to deal with more complex balance law for the entropy. This is the main source of the a-priori estimates, provided the model is consistent with the second law of thermodynamics. To ensure this, more general than usual forms of the transport fluxes must be considered. The mathematical investigation of such systems encounters various problems arising mostly due to a strong cross-diffusion in the species transport and the insufficient information about the density satisfying only the hyperbolic equation. Because of these difficulties, for a long time, the effort of mathematicians focused on systems simplifying either the reactive or dynamical aspects of the flow, or minimizing the coupling between them. They still can be used to model particular phenomena, but most of nowadays applications require more detailed description. For example, in modeling hydrogen-oxygen system included in a number of chemical mechanisms, as many as 20 different reactions can be taken into account involving the eight species:

$$H_2, \quad O_2, \quad H_2O, \quad OH, \quad O, \quad H, \quad HO_2 \text{ and } H_2O_2.$$
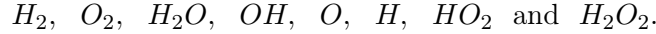
Moreover, depending upon the temperature, pressure, and extent of reaction, all the reverse reactions can become important [22].

The equations governing multicomponent reactive flow express the physical laws of conservation of mass, momentum, total energy and the balances of species mass, respectively:

$$\left. \begin{aligned} \partial_t\varrho + \operatorname{div}(\varrho\mathbf{u}) &= 0 \\ \partial_t(\varrho\mathbf{u}) + \operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u}) - \operatorname{div}\mathbf{S} + \nabla\pi &= \varrho\mathbf{f} \\ \partial_t(\varrho E) + \operatorname{div}(\varrho E\mathbf{u}) + \operatorname{div}(\pi\mathbf{u}) + \operatorname{div}\mathbf{Q} - \operatorname{div}(\mathbf{Su}) &= \varrho\mathbf{f}\cdot\mathbf{u} \\ \partial_t\varrho_k + \operatorname{div}(\varrho_k\mathbf{u}) + \operatorname{div}(\mathbf{F}_k) &= \varrho\vartheta\omega_k, \quad k\in\{1,...,n\} \end{aligned} \right\} \quad \text{in } (0,T)\times\Omega, \qquad (1)$$

were, $\mathbf{u}: \mathbb{R}^3 \to \mathbb{R}^3$ is the velocity field, $\varrho : \mathbb{R}^3 \to \mathbb{R}$ denotes the total mass density being a sum of species densities ϱ_k, $k \in \{1,\ldots,n\}$. The last unknown quantity is the temperature $\vartheta : \mathbb{R}^3 \to \mathbb{R}$ which appears implicitly in all the equations of (1) except for the continuity equation. Next, $\mathbf{S}$

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denotes the viscous stress tensor, the internal pressure is denoted by π, $\mathbf{f}$ is a given external force, E is the total energy per unit mass, which is a sum of internal energy e and the kinetic energy $\frac{\mathbf{u}^2}{2}$, $\mathbf{Q}$ stands for the heat flux, $\mathbf{F}_k$, $k \in \{1, \ldots, n\}$ denote the species diffusion fluxes and ω_k, $k \in \{1, \ldots, n\}$ are the chemical source terms, also termed the species production rates; $\Omega \subset \mathbb{R}^3$ and $T < +\infty$. Equivalently, the species mass conservation equations can be written in terms of species mass fractions Y_k, $k \in \{1, \ldots, n\}$ defined as $Y_k = \frac{\varrho_k}{\varrho}$.

The derivation of such model from the kinetic theory of gases can be found in numerous textbooks [7, 15, 23], for the alternative model – assigning densities and velocity fields to each species of the fluid – we refer to [21].

In order to close the system (1) one needs to supplement the field equations by the set of constitutive relations characteristic for viscous, heat-conducting and chemically-reacting mixtures. Since the list is considerably long, we focus only on these features of the system which appear in the context of global-in-time existence of weak solutions with no restriction for the size of initial data for the first time. More detailed discussion on this issue, depending on the purpose, can be found in the introductions to each of chapters of the thesis.

As already mentioned, the chemical composition of the mixture is taken into account in all thermodynamical quantities describing the system. In particular, we consider the pressure $\pi = \pi(\varrho, \vartheta, Y)$, which can be decomposed into $\pi = \pi_c + \pi_m$, where the first part is the barotropic pressure ϱ^γ, $\gamma > 1$, while the latter is the classical molecular pressure of the mixture determined through the *Boyle law* as a sum of partial pressures

$$\pi_m(\varrho, \vartheta, Y) = \sum_{k=1}^{n} p_k(\varrho, \vartheta, Y_k) = R \sum_{k=1}^{n} \frac{\vartheta \varrho Y_k}{m_k}, \tag{2}$$

with m_k – the molar mass of the k-th species and R – the perfect gas constant.
Naturally, we want the model to be consistent with the principles of continuum mechanics and thermodynamics. Especially, the concept of entropy is of great importance, as the second law of thermodynamics asserts that the entropy of any admissible process cannot decrease. An equation governing the entropy s can be deduced from system (1) by use of the Gibbs relation

$$\vartheta \mathrm{D}s = \mathrm{D}e + \pi \mathrm{D}\left(\frac{1}{\varrho}\right) - \sum_{k=1}^{n} g_k \mathrm{D}Y_k,$$

where $g_k(\varrho, \vartheta, Y)$ are the Gibbs functions and D denotes the total derivative, we have

$$\partial_t(\varrho s) + \mathrm{div}(\varrho s \mathbf{u}) + \mathrm{div}\left(\frac{\mathbf{Q}}{\vartheta} - \sum_{k=1}^{n} \frac{g_k}{\vartheta} \mathbf{F}_k\right) = \sigma,$$

where σ is the entropy production rate and it satisfies

$$\sigma = \underbrace{\frac{\mathbf{S} : \nabla \mathbf{u}}{\vartheta}}_{\geq 0} + \underbrace{\frac{\kappa |\nabla \vartheta|^2}{\vartheta^2}}_{\geq 0} - \underbrace{\sum_{k=1}^{n} g_k m_k \omega_k}_{\geq 0} - \underbrace{\sum_{k=1}^{n} \frac{\mathbf{F}_k}{m_k} \cdot \nabla \left(\log p_k\right)}_{\geq 0}. \tag{3}$$

Non-negativity of the first component follows from assumptions on the viscous stress tensor obeying the *Newton rheological law*, namely $\mathbf{S} = 2\mu \mathbf{D}(\mathbf{u}) + \nu \, \mathrm{div}\, \mathbf{u} \mathbb{I}$, where $\mathbf{D}(\mathbf{u}) = \frac{1}{2}\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right)$ and

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μ, ν are the Lamé viscosity coefficients $\mu > 0$, $2\mu + 3\nu \geq 0$. The second component in (3) is non-negative because the thermal conductivity coefficient is positive, $\kappa > 0$. Non-negativity of the third component is assumed as an admissibility condition for the chemical reaction to occur (cf. [15]). Finally, assuming the following form of the species diffusion fluxes

$$\mathbf{F}_k = -\sum_{k=1}^{n} C_{kl}\mathbf{d}_l, \qquad \mathbf{d}_k = \nabla\left(\frac{p_k}{\pi_m}\right) + \left(\frac{p_k}{\pi_m} - \frac{\varrho_k}{\varrho}\right)\nabla\log\pi_m, \tag{4}$$

where C_{kl} are multicomponent flux diffusion coefficients, we verify that the last component is also non-negative provided the matrix $D_{kl} = \frac{C_{kl}}{\varrho_k}$ has good properties. In our case it is symmetric ond positive definite over $U^{\perp}$ – the orthogonal complement of $lin(U)$, $U = (1, \ldots, 1)^T$, (see [15, 23]).

Here it should be emphasized that assuming the Fick approximation would lead to inconsistency with the second law of thermodynamics if the molecular pressure would be given by (2). In this case, the sign of the entropy production may fail to be non-negative, which contradicts physical admissibility of the process. This in turn interferes with obtaining the fundamental a-priori estimates causing that the energy methods break down.

The thesis consists of four main parts. Each of them is a distinct result based on the series of articles [18, 19, 24–26]. In Chapter 2 we examine the following reduction of system (1)

$$\left. \begin{aligned} \operatorname{div}(\varrho\mathbf{u}) &= 0 \\ \operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u}) - \operatorname{div}\mathbf{S} + \nabla\pi &= \varrho\mathbf{f} \\ \operatorname{div}(\varrho Y_A\mathbf{u}) + \operatorname{div}(\mathbf{F}_A) &= \varrho\omega_A \\ \operatorname{div}(\varrho Y_B\mathbf{u}) + \operatorname{div}(\mathbf{F}_B) &= \varrho\omega_B \\ \operatorname{div}(\varrho Y_C\mathbf{u}) + \operatorname{div}(\mathbf{F}_C) &= \varrho\omega_C \end{aligned} \right\} \text{ in } \Omega \tag{5}$$

governing the steady flow of four-component gaseous mixture undergoing an isothermal, reversible chemical reaction constituted by $A + B \rightleftharpoons C$, which takes place in the presence of a dilutant D. We supplement system (5) by the Dirichlet boundary condition for the velocity and by the impermeability conditions fort the species diffusion fluxes. Moreover, since there is no need to use the notion of the entropy, we assume that the species mass fluxes are given by the Fick law.

The main result of this chapter concerns the existence of weak solutions when the adiabatic exponent for the mixture γ is greater than $7/3$. The weak solution is constructed classically, by relaxation and elliptic regularization of the continuity equation, relaxation and regularization of the coefficients in the species mass balance equations in combination with the fixed point argument. The main difference, in comparison to the similar, but evolutionary and heat-conducting case, studied in [14], is that we cannot exclude the vacuum at any step of approximation procedure. Therefore, showing non-negativity of the species concentrations requires to consider also the case when $\varrho = 0$. The second part of the proof is the limit passage, in which we follow the idea of Lions [17] based on the DiPerna-Lions transport theory [9]. This approach requires the L^2 integrability of the density in order to get the renormalized solution of the continuity equation which is later on used to exploit *the effective viscous flux equality*. In the barotropic case it is possible to improve the value of γ be applying the oscillations defect measure introduced by Feireisl [10]. It seems, however, that here this technique could not be used due to presence of the molecular pressure.

In Chapter 3 we start to deal with vanishing viscosity coefficients satisfying the following relation

$$\nu(\varrho) = 2\varrho\mu'(\varrho) - 2\mu(\varrho), \tag{6}$$

introduced by Bresch and Desjardins in [3]. The main difficulty in comparison to the systems with viscosity coefficients bounded from below by a constant [12, 17], is lack of information about the velocity vector field. Although this degeneracy causes additional difficulties, it also contributes some benefits, if only relation (6) is satisfied. It provides particular mathematical structure that yields boundedness of $\nabla\sqrt{\varrho}$. This property was observed for the first time by Bresch, Desjardins and Lin [6] for the Korteweg equations and for the 2-dimensional viscous shallow water model [2]. Later on, Mellet and Vasseur coupled this idea with the additional estimate for the norm of $\varrho\mathbf{u}^2$ in $L^\infty(0, T; L\log L(\Omega))$ and proved the sequential stability of weak solutions to the barotropic compressible Navier-Stokes system.

Assuming (6), we investigate the system of equations describing flow of two-component isothermal gaseous mixture in the periodic domain $\Omega = \mathbb{T}^3$. At first sight this situation seems to be simpler, than the one considered in the previous chapter, however, now our main aim is to investigate the cross-diffusion phenomenon occurring in majority of multicomponent flows. We focus on a simplest form of the diffusion matrix C, which does not lead to inconsistency with the second law of thermodynamics when the heat-conductivity is included. But even in this case, one has to face the problem of appearance of a new type of degeneration in the species equations caused by the form of diffusion fluxes

$$\mathbf{F}_i = -C_0\mathbf{d}_i = -\frac{C_0}{\pi_m}\left(\left(\frac{\varrho_k}{\varrho m_i} + \frac{\varrho_i}{\varrho m_k}\right)\nabla\varrho_i - \frac{\varrho_i}{\varrho m_k}\nabla\varrho\right), \quad i \neq k.$$

The first part of this chapter is devoted to the proof of sequential stability of weak solutions. The main observation here is that the missing information about the species densities may be compensated by the higher regularity of the density deduced from the additional estimate involving relation (6). Although the stability result is widely regarded as a most difficult part, the compete proof of existence of solutions in this framework is still elusive. The main difficulty is to preserve the logarithmic estimate for the velocity, yielding convergence in the convective term, at any level of construction of solution. To the best of our knowledge, when no additional drag terms are present, this is still an open problem, even for the barotropic case.

In the second part of the chapter we give a detailed description of the approximate scheme and prove the existence of weak solutions for arbitrary large initial data, under further assumption on the barotropic pressure. By this modification, the compactness of the sequence approximating the velocity can be shown with no effort. So, in order to construct the approximate solution, one needs only to preserve the structure allowing to maintain an extra estimate of the density. The basic idea is contained already in the work [4] and consists of introducing the smoothing operator $\delta\varrho\nabla\left(\mu'(\varrho)\Delta^{2s+1}\mu(\varrho)\right)$ with s sufficiently large, inspired from the capillarity forces [6]. In the next step we improve regularity of velocity using the biharmonic operator $\eta\Delta^2\mathbf{u}$. Finally, to get the estimate for the norm of $\Delta^{s+1}\varrho$ in $L^2((0, T) \times \Omega)$ at the level of Faedo-Galerkin approximation, we also need to regularize the the continuity equation, and hence, the species equations, by adding $\varepsilon\Delta\varrho$.

In Chapter 4 we investigate only the reaction-diffusion equations of species keeping the thermodynamical framework originating from the general theory of mixtures. Our main achievement is the proof of existence of weak solutions for arbitrary number of reacting species under the assumption that the total density is as regular as it follows from the previous chapter. Our result has three possible interpretations:

- For the simplest case $\mathbf{u} \equiv \mathbf{0}$ the density ϱ is a given fixed function and the model takes into account just diffusion, neglecting the effects of transport.

- If the velocity field is given, the chemical reactions have no influence on the speed of particles, they do not produce any internal force (pressure like force). Such model is admissible for "cold" reactions, where we do not observe any rapid changes of energy.

- If the system of reaction-diffusion equations is a part of the full model (1), then our result can be viewed as an auxiliary tool giving hints how to proceed with the full system.

Note that we are able to handle the nonlinear terms appearing in all the species diffusion forces $\mathbf{d}_k$, $k \in \{1, \ldots, n\}$, while the matrix of diffusion coefficients C_{kl} satisfies all the general assumptions from [15], Chapter 7. This is, however, the main obstacle to apply the classical approach for systems of parabolic equations [1, 8, 16]. Indeed, although the diffusion fluxes form an elliptic operator it is not diagonal, not even symmetric. Thus, any direct technique of renormalization of the system is not admissible as it is the case for the scalar systems [20]. The only possibility is to employ the information about the entropy production (3), then we deal with the symmetric matrix D_{kl} which is positive definite but only over a subspace of co-dimension 1. It follows that the whole mathematical analysis should be done in terms of $\log p_k$ instead of ϱ_k. This approach is effective, since it guarantees immediately that the densities of gas components will be nonnegative. Using a suitable approximation we are allowed to obtain existence through the Galerkin approximation, and then passing to subsequent limits, we find the solution of the original problem. The compactness of the approximative sequence is guaranteed due to uniform $L \log L$ bounds and an extra information about the whole density ϱ. The last fact allows to control the regularity of space derivatives of solutions.

The purpose of the last chapter is to bring together and complement the previous results in order to treat the complete mathematical model governing the motion of n-component, heat-conducting reactive gaseous mixture. We prove sequential stability of *weak variational entropy solutions* for the same modification of the barotropic pressure as in [26] and when the species diffusion fluxes depend on the gradients of partial pressures, analogously as in [19]. Of crucial importance for our analysis is again the fact that viscosity coefficients are related by (6) and the source terms enjoy the admissibility condition dictated by the second law of thermodynamics. Thanks to this, we are able to combine the entropy inequality with the Bresch-Desjardins type of estimate [5]. The latter allows us to regain the part of regularity of the species densities which, due to a multicomponent diffusion (4), is not a-priori available. However, the presence of the temperature causes that the method scratched in [26] and [19] is now more intricate.

It is to be noticed that, unlike to [5], we perform the limit passage in the framework of weak variational entropy formulation. For the Navier-Stokes-Fourier system the concept of the weak variational entropy solution (i.e. a solution satisfying the balance of mass, momentum, the entropy inequality and the global balance of total energy) was introduced by Feireisl and Novotný, who proved the sequential stability [11] and the global-in-time existence of these solutions [12]. This result was then generalized by Feireisl, Petzeltová and Trivisa [14] to the case of chemically reacting flows, when there is no interaction among the species diffusion fluxes and the pressure does not depend on the chemical composition of the mixture.

What is still lacking to end up with the usual weak solution, is better regularity of the temperature required to pass to the limit in the internal energy balance. Also because of this, compactness (with respect to time) of the sequence approximating the temperature, could not be deduced directly from the energy equation. The last problem was solved by applying the compensated compactness methods to the entropy inequality.

Naturally, the main motivation to study the sequential stability of weak solutions is to obtain the complete existence result. It seems to be a very complex and technically complicated task, even if the correction of the pressure is postulated, and it is left for the future study.

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