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# DIFFUSION MODELS FOR MIXTURES USING A STIFF DISSIPATIVE HYPERBOLIC FORMALISM

LAURENT BOUDIN, BÉRÉNICE GREC, AND VINCENT PAVAN

ABSTRACT. In this article, we are interested in a system of fluid equations for mixtures with a stiff relaxation term of Maxwell-Stefan diffusion type. We use the formalism developed by Chen, Levermore, Liu in [4] to obtain a limit system of Fick type where the species velocities tend to align to a bulk velocity when the relaxation parameter remains small.

## 1. INTRODUCTION AND MOTIVATIONS

In this work, we consider a system of fluid equations for mixtures with a stiff diffusion term of Maxwell-Stefan type. This system was introduced in various works such as [10] (see also the references therein). It was also derived in [2], using the kinetic theory toolbox to derive the values of the diffusion coefficients with respect to microscopic quantities. We consider an ideal gas mixture with  $p \geq 2$  species evolving in a subset  $\Omega$  of  $\mathbb{R}^d$ ,  $d \geq 1$ . The system under study reads, for  $1 \leq i \leq p$

$$(1) \quad \partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i) = 0, \quad \mathbf{x} \in \mathbb{R}^d, t \geq 0,$$

$$(2) \quad \partial_t (\rho_i \mathbf{u}_i) + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i) + \nabla_{\mathbf{x}} P_i(\rho_i) + \frac{1}{\varepsilon} \mathbf{R}_i = 0, \quad \mathbf{x} \in \mathbb{R}^d, t \geq 0,$$

where  $\varepsilon > 0$  is the small relaxation time parameter, and, for any  $1 \leq i \leq p$ ,  $\rho_i > 0$  denotes the mass density of species  $i$ ,  $\rho_i \mathbf{u}_i \in \mathbb{R}^d$  its momentum, and both depend on  $\mathbf{x}$  and  $t$ . The partial pressure  $P_i(\rho_i)$  of species  $i$  in the mixture can be expressed in terms of the mass density  $\rho_i$ . More precisely, it writes, thanks to the ideal gas law,  $P_i(\rho_i) = \rho_i k_B T / m_i$ , where  $m_i$  is the molecular mass of species  $i$ ,  $T$  the mixture temperature, assumed to be constant and  $k_B$  the Boltzmann constant.

The relaxation term  $\mathbf{R}_i$  is a friction force exerted by the mixture on species  $i$ . It is given by

$$\mathbf{R}_i = \sum_{j \neq i} \alpha_{ij} (\mathbf{u}_j - \mathbf{u}_i),$$

where  $\alpha_{ij} \geq 0$  for any  $i \neq j$ . This implies that  $\mathbf{R}_i$  has an alignment effect on the species velocities  $\mathbf{u}_i$ , which is classical for modelling mixtures (see [10] for instance), in particular when focusing on the diffusive parts of the model. The sign of  $\alpha_{ij}$  was formally proven in [2], as well as the symmetry property  $\alpha_{ij} = \alpha_{ji}$ . Moreover, each  $\alpha_{ij}$  can be written under the form  $\alpha_{ij} = a_{ij} \rho_i \rho_j$ , where  $a_{ij} > 0$  mainly depends on the molecular masses of species  $i$  and  $j$ , and on the mixture temperature. The values  $\alpha_{ij}$  are linked to the binary diffusion coefficients appearing in the Maxwell-Stefan diffusion equations [5, 9, 1, 3, 7].

Let us set, for  $1 \leq i \leq p$ ,

$$(3) \quad \alpha_{ii} = - \sum_{j \neq i} \alpha_{ij}.$$

Then the symmetric matrix  $\mathbb{A} = (\alpha_{ij})_{1 \leq i, j \leq p}$  is nonnegative semi-definite, with rank  $p - 1$ , and its null space  $\ker \mathbb{A}$  is spanned by  $(1, \dots, 1)^\top \in \mathbb{R}^p$ , as stated in [2].

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Equations (1)–(2) clearly constitute a system of hyperbolic conservation laws with a stiff relaxation term. Our work adapts the argument developed in [4] in the gaseous mixture framework. We aim to derive an approximation of the local equilibrium and its first-order correction. To do so, we build a relevant entropy, as explained, for instance in [6], which ensures the hyperbolicity of the local equilibrium approximation and the dissipativity of the first-order correction term. Then we deduce a reduced system on the conserved quantities. Consequently, we benefit from the general setting introduced in [4]. This setting was widely studied from a rigorous mathematical viewpoint. Yong first built [12] a singular perturbation theory to justify the asymptotic expansion, if one assumes the existence of smooth solutions to the reduced system. Then the existence of global smooth solutions to such systems of hyperbolic conservation laws was obtained in [8, 13] under suitable stability conditions.

In our case, applying Chen, Levermore and Liu’s [4] formalism allows us to obtain a reduced system involving the aligned velocity  $\mathbf{u}$  when  $\varepsilon$  remains small, as stated in the following proposition.

**Proposition 1.** *System (1)–(2) formally reduces to the following equations*

$$(4) \quad \partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}) = \varepsilon \nabla_{\mathbf{x}} \cdot \left( \sum_{j=1}^p \ell_{ij} \frac{\nabla_{\mathbf{x}} P_j}{\rho_j} \right), \quad 1 \leq i \leq p,$$

$$(5) \quad \partial_t (\rho \mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} P = \mathbf{0},$$

where  $\mathbf{u}$  is the mass-weighted average velocity of the mixture,  $P = \sum_j P_j(\rho_j)$  is the total pressure, and the matrix  $(\ell_{ij})_{1 \leq i, j \leq p}$  is symmetric non-positive.

Let us briefly comment the structure of System (4)–(5). Equations (4) provide the mass conservation laws on each species. The right-hand sides are indeed of diffusive nature in the isothermal setting: since each species is an ideal gas, then  $P_j$  is proportional to  $\rho_j$ , and the term  $\nabla_{\mathbf{x}} P_j / \rho_j$  can be interpreted as a simplified writing of  $\nabla_{\mathbf{x}} (\mu_j / T)$ , where  $\mu_j$  is the chemical potential of species  $j$ , which arises in thermodynamics of irreversible processes point of view. In fact, the matrix of coefficients  $(\ell_{ij})$ , obtained as a relevant pseudo-inverse of  $\mathbb{A}$ , allows to recover the diffusion matrix appearing in the Fick diffusion equations. The diffusive part of the molar/mass fluxes of each species appears as a correction of order  $\varepsilon$  to the main convective flux, as suggested by Chen, Levermore and Liu. Equation (5) is the only one available on the momentum, it involves the total momentum of the mixture, and it does not include any terms of order  $\varepsilon$ .

Before applying Chen, Levermore and Liu’s formalism, we first need to enlighten the reader about the article notations for tensors and vectors. For instance,  $\mathbf{W}$  will denote a quantity which must be treated as a tensor, whereas  $W$  is a constant and  $\mathbf{W}$  must be considered as a vector in the physical space  $\mathbb{R}^d$ . Moreover,  $\mathbb{I}_q$  is the identity matrix of size  $q \in \mathbb{N}^*$ ,  $\mathbf{0}_{p \times q}$  is the zero matrix of size  $p \times q$ , and  $\mathbf{1}_{p \times q}$  is the matrix of size  $p \times q$  filled with ones, for  $p, q \in \mathbb{N}^*$ .

Let us set

$$(6) \quad \mathbf{W} = \begin{bmatrix} W_1 \\ \vdots \\ W_p \\ \mathbf{W}_{p+1} \\ \vdots \\ \mathbf{W}_{2p} \end{bmatrix} \in \mathbb{R}^{p+dp},$$

where the components of  $\mathbf{W}$  appearing in (6) are given by

$$(7) \quad W_i = \rho_i, \quad \mathbf{W}_{p+i} = \rho_i \mathbf{u}_i, \quad 1 \leq i \leq p.$$

Then the vector-valued unknown function  $\mathbf{W}$  solves the following evolutionary partial differential equation

$$(8) \quad \partial_t \mathbf{W} + \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{W}) + \frac{1}{\varepsilon} \mathbf{R}(\mathbf{W}) = 0,$$

where both the flux  $\mathbf{F}(\mathbf{W})$  and relaxation  $\mathbf{R}(\mathbf{W})$  tensor terms have to be clarified. Note that, in fact,  $\mathbf{W}$  lies in  $(\mathbb{R}_+)^p \times \mathbb{R}^{dp}$ . Moreover, the mass densities  $W_i(t, x)$ ,  $1 \leq i \leq p$ , are supposed to remain positive for  $t > 0$  and  $x \in \mathbb{R}^d$ .

In order to properly write the flux  $\mathbf{F}(\mathbf{W}) \in \mathbb{R}^{(p+dp) \times d}$ , let us denote by  $(\mathbf{e}_k)_{1 \leq k \leq d}$  the natural basis of  $\mathbb{R}^d$ . Then the  $k$ -th column,  $1 \leq k \leq d$ , of  $\mathbf{F}(\mathbf{W})$  is given by

$$\mathbf{F}_k(\mathbf{W}) = \begin{bmatrix} \mathbf{F}_k^1(\mathbf{W}) \\ \mathbf{F}_k^2(\mathbf{W}) \end{bmatrix} \in \mathbb{R}^{p+dp},$$

with

$$\begin{aligned} \mathbf{F}_k^1(\mathbf{W}) &= \begin{bmatrix} \mathbf{W}_{p+1} \cdot \mathbf{e}_k \\ \vdots \\ \mathbf{W}_{2p} \cdot \mathbf{e}_k \end{bmatrix} \in \mathbb{R}^p, \\ \mathbf{F}_k^2(\mathbf{W}) &= \begin{bmatrix} \left( \frac{\mathbf{W}_{p+1} \otimes \mathbf{W}_{p+1}}{W_1} + P_1(W_1) \mathbb{I}_d \right) \mathbf{e}_k \\ \vdots \\ \left( \frac{\mathbf{W}_{2p} \otimes \mathbf{W}_{2p}}{W_p} + P_p(W_p) \mathbb{I}_d \right) \mathbf{e}_k \end{bmatrix} \in \mathbb{R}^{dp}. \end{aligned}$$

As we mentioned it before, the species involved in the mixture are assumed to be ideal gases, so that, for any  $1 \leq i \leq p$ , the pressure law for species  $i$  reads

$$(9) \quad P_i(W_i) = \frac{W_i k_B T}{m_i}.$$

Finally, the relaxation term  $\mathbf{R}(\mathbf{W})$  is given by

$$\mathbf{R}(\mathbf{W}) = \begin{bmatrix} \mathbf{0}_{p \times 1} \\ \sum_{j \neq 1} \alpha_{1j} \left( \frac{\mathbf{W}_{p+j}}{W_j} - \frac{\mathbf{W}_{p+1}}{W_1} \right) \\ \vdots \\ \sum_{j \neq p} \alpha_{pj} \left( \frac{\mathbf{W}_{p+j}}{W_j} - \frac{\mathbf{W}_{2p}}{W_p} \right) \end{bmatrix} \in \mathbb{R}^{p+dp}.$$

With the definition (3) of  $\alpha_{ii}$  we chose, we can rewrite the previous expression of  $\mathbf{R}$  as

$$\mathbf{R}(\mathbf{W}) = \begin{bmatrix} \mathbf{0}_{p \times 1} \\ \sum_{j=1}^p \alpha_{1j} \frac{\mathbf{W}_{p+j}}{W_j} \\ \vdots \\ \sum_{j=1}^p \alpha_{pj} \frac{\mathbf{W}_{p+j}}{W_j} \end{bmatrix} \in \mathbb{R}^{p+dp}.$$

Eventually, let us point out that the methodology of [4] is very close to strategies involving the Chapman-Enskog or Hilbert expansions, classically used in kinetic theory to derive hydrodynamic equations from the Boltzmann equation. The analogous of  $\mathbf{W}$  would then be the distribution function, the friction relaxation term  $\mathbf{R}$  the collision operator with the same kind of dissipativity and collisional invariant properties, and of course the local equilibria the Maxwell functions. Note that [11] presents a validity proof of such an expansion in a more general physical setting (non-ideal thermochemistry).

The article is structured as follows. In Section 2, we construct the entropy and compute the local equilibria. Then, in Section 3, by studying the relaxation term, we obtain the first-order correction and the reduced system.

## 2. ENTROPY AND EQUILIBRIUM

**2.1. Building the entropy.** The existence of a strictly convex entropy is a simple criterion to ensure the local equilibrium hyperbolicity and the first-order correction dissipativity property. More precisely, as stated in [4, Definition 2.1], such an entropy is a twice-differentiable function  $\eta : (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp} \rightarrow \mathbb{R}$  satisfying, for all  $\mathbf{W} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp}$ ,

$$(10) \quad \nabla_{\mathbf{W}}^2 \eta(\mathbf{W}) \nabla_{\mathbf{W}} F_k(\mathbf{W}) \text{ is symmetric for any } 1 \leq k \leq d,$$

$$(11) \quad \nabla_{\mathbf{W}} \eta(\mathbf{W}) \cdot \mathbf{R}(\mathbf{W}) \geq 0,$$

$$(12) \quad \nabla_{\mathbf{W}}^2 \eta(\mathbf{W}) \text{ is a positive definite quadratic form.}$$

A natural choice for  $\eta$  in our setting is the total energy of the mixture, obtained as the sum of both kinetic and internal energies of each species. The internal energy  $E_i(W_i)$  of species  $i$ ,  $1 \leq i \leq p$ , can be defined thanks to

$$(13) \quad E_i''(W_i) = \frac{P_i'(W_i)}{W_i}.$$

This choice will ensure the symmetry condition (10). Taking (9) into account, that leads, for instance, to

$$(14) \quad E_i'(W_i) = \frac{k_B T}{m_i} \ln \left( \frac{W_i}{W_i^0} \right), \quad E_i(W_i) = \frac{k_B T}{m_i} \left( W_i \ln \left( \frac{W_i}{W_i^0} \right) - W_i \right),$$

where  $W_i^0 > 0$  is an arbitrary constant. Then it is possible to define the entropy with the following proposition.

**Proposition 2.** *The function  $\eta$  defined by*

$$(15) \quad \eta : (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp} \rightarrow \mathbb{R}, \quad \mathbf{W} \mapsto \sum_{i=1}^p \frac{1}{2} \frac{W_i^2}{W_i} + E_i(W_i)$$

*is a strictly convex entropy for Equation (8).*

Before starting the proof of the previous proposition, we need to introduce a very convenient notation for block diagonal matrices.

**Notation 1.** *For any  $q, r, s \in \mathbb{N}^*$  and any matrices  $M_i \in \mathbb{R}^{r \times s}$ ,  $1 \leq i \leq q$ , we define the block matrix*

$$\text{Diag}_{qr \times qs}(M_i) = \begin{bmatrix} M_1 & & & \\ & M_2 & & \\ & & \ddots & \\ & & & M_q \end{bmatrix} \in \mathbb{R}^{qr \times qs}.$$

*Let us point out that index  $i$  in the notation refers to the generic block index of the matrix on the diagonal.*

*Proof.* Let us now prove Proposition 2 by checking (10)–(12). We first perform the preliminary computations of  $\nabla_{\mathbf{W}}\eta(\mathbf{W})$  and  $\nabla_{\mathbf{W}}^2\eta(\mathbf{W})$ . From (15), it is easy to obtain

$$(16) \quad \nabla_{\mathbf{W}}\eta(\mathbf{W}) = \left[ -\frac{\mathbf{W}_{p+1}^2}{2W_1^2} + E'_1(W_1), \dots, -\frac{\mathbf{W}_{2p}^2}{2W_p^2} + E'_p(W_p), \frac{\mathbf{W}_{p+1}^\top}{W_1}, \dots, \frac{\mathbf{W}_{2p}^\top}{W_p} \right]^\top$$

and thereafter

$$\nabla_{\mathbf{W}}^2\eta(\mathbf{W}) = \begin{bmatrix} \text{Diag}_{p \times p} \left( \frac{\mathbf{W}_{p+i}^2}{W_i^3} + E''_i(W_i) \right) & -\text{Diag}_{p \times dp} \left( \frac{\mathbf{W}_{p+i}^\top}{W_i^2} \right) \\ -\text{Diag}_{dp \times p} \left( \frac{\mathbf{W}_{p+i}}{W_i^2} \right) & \text{Diag}_{dp \times dp} \left( \frac{\mathbb{I}_d}{W_i} \right) \end{bmatrix}.$$

*Checking (12).* The strict convexity of  $\eta$  is then clear, since, if we set

$$\mathbf{X} = [X_1, \dots, X_p, \mathbf{X}_{p+1}^\top, \dots, \mathbf{X}_{2p}^\top]^\top \in \mathbb{R}^{p+dp},$$

then

$$\nabla_{\mathbf{W}}^2\eta(\mathbf{W})\mathbf{X} \cdot \mathbf{X} = \sum_{i=1}^p \left[ \left( \frac{\mathbf{W}_{p+i}^2}{W_i^3} + E''_i(W_i) \right) X_i^2 + \frac{1}{W_i} \mathbf{X}_{p+i}^2 \right],$$

which is clearly positive if  $\mathbf{X} \neq 0$ . Note that the off-diagonal terms of the Hessian of  $\eta$  cancel in the previous computation.

*Checking (10).* The vector  $\nabla_{\mathbf{W}}\mathbf{F}_k(\mathbf{W})$  is computed as

$$(17) \quad \begin{aligned} \nabla_{\mathbf{W}}\mathbf{F}_k(\mathbf{W}) &= [\nabla_{\mathbf{W}}\mathbf{F}_k^1(\mathbf{W}) \quad \nabla_{\mathbf{W}}\mathbf{F}_k^2(\mathbf{W})]^\top \\ &= \begin{bmatrix} \mathbf{0}_{p \times p} & \text{Diag}_{p \times dp}(\mathbf{e}_k^\top) \\ \text{Diag}_{dp \times p} \left( \left[ -\frac{\mathbf{W}_{p+i} \otimes \mathbf{W}_{p+i}}{W_i^2} + P'_i(W_i)\mathbb{I}_d \right] \mathbf{e}_k \right) & \text{Diag}_{dp \times dp} \left( \frac{\mathbf{W}_{p+i} \cdot \mathbf{e}_k}{W_i} \mathbb{I}_d + \frac{\mathbf{W}_{p+i} \otimes \mathbf{e}_k}{W_i} \right) \end{bmatrix}. \end{aligned}$$

The matrix product  $\nabla_{\mathbf{W}}^2\eta(\mathbf{W})\nabla_{\mathbf{W}}\mathbf{F}_k(\mathbf{W})$  then provides

$$\begin{bmatrix} \text{Diag}_{p \times p} \left( \frac{\mathbf{W}_{p+i}^2}{W_i^4} - \frac{P'_i(W_i)}{W_i^2} \mathbf{W}_{p+i} \cdot \mathbf{e}_k \right) & \text{Diag}_{p \times dp} \left( E''_i(W_i)\mathbf{e}_k^\top - \frac{\mathbf{W}_{p+i} \cdot \mathbf{e}_k}{W_i^3} \mathbf{W}_{p+i}^\top \right) \\ \text{Diag}_{dp \times p} \left( \frac{P'_i(W_i)}{W_i} \mathbf{e}_k - \frac{\mathbf{W}_{p+i} \cdot \mathbf{e}_k}{W_i^3} \mathbf{W}_{p+i} \right) & \text{Diag}_{dp \times dp} \left( \frac{\mathbf{W}_{p+i} \cdot \mathbf{e}_k}{W_i^2} \mathbb{I}_d \right) \end{bmatrix},$$

the symmetry of which is ensured because of (13).

*Checking (11).* We compute

$$(18) \quad \nabla_{\mathbf{W}}\eta(\mathbf{W}) \cdot \mathbf{R}(\mathbf{W}) = \sum_{i,j} \alpha_{ij} \frac{\mathbf{W}_{p+i}}{W_i} \cdot \frac{\mathbf{W}_{p+j}}{W_j} = \sum_{k=1}^d \left[ \sum_{i,j} \alpha_{ij} \frac{\mathbf{W}_{p+i} \cdot \mathbf{e}_k}{W_i} \frac{\mathbf{W}_{p+j} \cdot \mathbf{e}_k}{W_j} \right],$$

which is clearly nonnegative for any  $\mathbf{W}$ , since the matrix  $\mathbf{A} = (\alpha_{ij})$  is known to be nonnegative.

That concludes the proof of Proposition 2.  $\square$

**2.2. Definition and properties of the local equilibria.** Let us first introduce the following matrix

$$\mathbb{Q} = \begin{bmatrix} \mathbb{I}_p & \mathbf{0}_{p \times dp} \\ \mathbf{0}_{d \times p} & \mathbb{Q}_{22} \end{bmatrix} \in \mathbb{R}^{(p+d) \times (p+dp)},$$

where

$$\mathbb{Q}_{22} = [\mathbb{I}_d, \dots, \mathbb{I}_d] \in \mathbb{R}^{d \times dp}.$$

Observe that for any  $\mathbf{W} \in \mathbb{R}^{p+d}$ ,  $\mathbb{Q}\mathbf{W}$  is given by

$$\mathbb{Q}\mathbf{W} = \left[ W_1, \dots, W_p, \sum_{j=1}^p \mathbf{W}_{p+j}^\top \right]^\top.$$

The relaxation term  $\mathbf{R}$  is a vector field which has  $p + d$  independent linear conserved quantities. Those quantities can be described thanks to  $\mathbb{Q}$ , since  $\mathbb{Q}\mathbf{R}(\mathbf{W}) = \mathbf{0}_{(p+d) \times 1}$  and the null space of  $\mathbb{Q}$ , given by

$$(19) \quad \ker \mathbb{Q} = \left\{ \left[ 0, \dots, 0, \mathbf{W}_{p+1}^\top, \dots, \mathbf{W}_{2p}^\top \right]^\top, \sum_{j=1}^p \mathbf{W}_{p+j} = \mathbf{0}_{d \times 1} \right\},$$

indeed satisfies  $\dim \ker \mathbb{Q} = d(p - 1)$ .

Any  $\mathbf{W}_{\text{eq}} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp}$  is called a local equilibrium if  $\mathbf{R}(\mathbf{W}_{\text{eq}}) = \mathbf{0}$ . These equilibria are characterized in the following way.

**Proposition 3.** *The following properties are equivalent:*

- (i)  $\mathbf{W}$  is a local equilibrium,
- (ii)  $\nabla_{\mathbf{W}}\eta(\mathbf{W}) \cdot \mathbf{R}(\mathbf{W}) = 0$ ,
- (iii) there exists  $\mathbf{u} \in \mathbb{R}^d$  such that  $\mathbf{W}$  has the form

$$(20) \quad \mathbf{W} = [W_1, \dots, W_p, W_1\mathbf{u}^\top, \dots, W_p\mathbf{u}^\top]^\top,$$

- (iv) there exists  $\mathbf{v} \in \mathbb{R}^{p+d}$  such that  $\nabla_{\mathbf{W}}\eta(\mathbf{W}) = \mathbf{v}^\top \mathbb{Q}$ .

*Proof.* The equivalences of this proposition are decomposed into several implications in the proof, enough to ensure the equivalence between all the statements. The implication (i)  $\Rightarrow$  (ii) is straightforward.

*Checking (ii)  $\Rightarrow$  (iii).* Since the matrix  $\mathbb{A}$  has a one-dimensional null space spanned by  $\mathbf{1}_{p \times 1}$ , the term (18) equals zero if there exists  $\mathbf{u} \in \mathbb{R}^d$  such that

$$\frac{\mathbf{W}_{p+i} \cdot \mathbf{e}_k}{W_i} = \mathbf{u} \cdot \mathbf{e}_k, \quad 1 \leq k \leq d, \quad 1 \leq i \leq p.$$

*Checking (iii)  $\Rightarrow$  (iv).* Since there exists  $\mathbf{u} \in \mathbb{R}^d$  satisfying (20), it follows from (16) that

$$\nabla_{\mathbf{W}}\eta(\mathbf{W}) = \left[ -\frac{\mathbf{u}^2}{2} + E'_1(W_1), \dots, -\frac{\mathbf{u}^2}{2} + E'_p(W_p), \mathbf{u}^\top, \dots, \mathbf{u}^\top \right]^\top.$$

Let us consider the vector  $\mathbf{v}$  such that

$$\mathbf{v}^\top = \left[ -\frac{\mathbf{u}^2}{2} + E'_1(W_1), \dots, -\frac{\mathbf{u}^2}{2} + E'_p(W_p), \mathbf{u}^\top \right].$$

Then it is clear that  $\nabla_{\mathbf{W}}\eta(\mathbf{W}) = \mathbf{v}^\top \mathbb{Q}$ .

*Checking (iv)  $\Rightarrow$  (ii).* If  $\nabla_{\mathbf{W}}\eta(\mathbf{W}) = \mathbf{v}^\top \mathbb{Q}$  for some  $\mathbf{v} \in \mathbb{R}^{p+d}$ , then, since  $\mathbb{Q}\mathbf{R}(\mathbf{W}) = \mathbf{0}$ ,

$$\nabla_{\mathbf{W}}\eta(\mathbf{W}) \cdot \mathbf{R}(\mathbf{W}) = \mathbf{v}^\top \mathbb{Q}\mathbf{R}(\mathbf{W}) = 0.$$

Checking (iii)  $\Rightarrow$  (i). If there exists  $\mathbf{u} \in \mathbb{R}^d$  such that  $\mathbf{W}$  has the form

$$\mathbf{W} = [W_1, \dots, W_p, W_1 \mathbf{u}^\top, \dots, w_p \mathbf{u}^\top]^\top,$$

then, thanks to (3),

$$\mathbf{R}(\mathbf{W}) = \begin{bmatrix} 0_{p \times 1} \\ \left( \sum_{j=1}^p \alpha_{1j} \right) \mathbf{u} \\ \vdots \\ \left( \sum_{j=1}^p \alpha_{pj} \right) \mathbf{u} \end{bmatrix} = \mathbf{0}_{(p+dp) \times 1}.$$

This concludes the proof of Proposition 3.  $\square$

In order to determine the local equilibria, we first recall the definition and some properties of the Legendre-Fenchel transform of the entropy. We introduce the following domain

$$\mathcal{V} = \left\{ \mathbf{V} \in \mathbb{R}^{p+dp} \mid \mathbf{V} = \nabla_{\mathbf{W}} \eta(\mathbf{W}) \text{ for some } \mathbf{W} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp} \right\}.$$

Note that if  $\mathbf{V} \in \mathcal{V}$ , the associated  $\mathbf{W}$  satisfies  $W_i > 0$  for any  $1 \leq i \leq p$ . The Legendre-Fenchel transform  $\eta^*$  of  $\eta$  on the domain  $\mathcal{V}$  is the convex function satisfying

$$\eta(\mathbf{W}) + \eta^*(\mathbf{V}) = \mathbf{V} \cdot \mathbf{W}.$$

Taking the expressions (16) of  $\nabla_{\mathbf{W}} \eta(\mathbf{W})$  and (14) of  $E'_i$  into account, the definition of the elements  $\mathbf{V}$  of  $\mathcal{V}$  leads to

$$(21) \quad V_i = -\frac{\mathbf{W}_{p+i}^2}{2W_i^2} + \frac{k_B T}{m_i} \ln \left( \frac{W_i}{W_i^0} \right), \quad \mathbf{V}_{p+i} = \frac{W_i}{\mathbf{W}_{p+i}}, \quad 1 \leq i \leq p.$$

From (21), we deduce

$$W_i = W_i^0 \exp \left( \frac{m_i}{k_B T} \left( V_i + \frac{1}{2} \mathbf{V}_{p+i}^2 \right) \right) > 0.$$

Consequently, we compute  $\eta^*(\mathbf{V})$

$$(22) \quad \eta^*(\mathbf{V}) = \mathbf{V} \cdot \mathbf{W} - \eta(\mathbf{W}) = \sum_{i=1}^p \frac{k_B T}{m_i} W_i^0 \exp \left( \frac{m_i}{k_B T} \left( V_i + \frac{1}{2} \mathbf{V}_{p+i}^2 \right) \right).$$

**Proposition 4.** *The quantity  $\mathbf{W}$  is a local equilibrium if and only if there exists  $\mathbf{v} \in \mathbb{R}^{p+d}$  such that  $\mathbf{W} = \nabla_{\mathbf{V}} \eta^*(\mathbf{v}^\top \mathbf{Q})$ .*

*Proof.* Since

$$\nabla_{\mathbf{V}} \eta^*(\mathbf{V}) = \mathbf{W}, \quad \forall \mathbf{V} \in \mathcal{V} \quad \text{and} \quad \nabla_{\mathbf{W}} \eta(\mathbf{W}) = \mathbf{V}, \quad \forall \mathbf{W} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp},$$

the equivalence is straightforward.  $\square$

We are now in the position to explicitly compute the local equilibria.

**Proposition 5.** *The equilibrium function  $\mathcal{E} : (\mathbb{R}_+^*)^p \times \mathbb{R}^d \rightarrow \mathbb{R}^{p+dp}$ ,  $\mathbf{w} = (w_1, \dots, w_p, \mathbf{w}_{p+1}) \mapsto \mathcal{E}(\mathbf{w})$  is given by*

$$(23) \quad \mathcal{E}(\mathbf{w}) = \left[ w_1, \dots, w_p, \frac{w_1}{\sigma(\mathbf{w})} \mathbf{w}_{p+1}^\top, \dots, \frac{w_p}{\sigma(\mathbf{w})} \mathbf{w}_{p+1}^\top \right]^\top,$$

where  $\sigma(\mathbf{w}) = \sum_{i=1}^p w_i$ .



*Proof.* Let  $\phi^* : \mathbb{R}^{p+d} \rightarrow \mathbb{R}$ ,  $\mathbf{v} \mapsto \eta^*(\mathbf{v}^\top \mathbb{Q})$ . It is clear from (22) that

$$(24) \quad \phi^*(\mathbf{v}) = \sum_{i=1}^p \frac{k_B T}{m_i} W_i^0 \exp\left(\frac{m_i}{k_B T} \left(v_i + \frac{1}{2} \mathbf{v}_{p+1}^2\right)\right).$$

Denote by  $\phi$  the Legendre-Fenchel transform of  $\phi^*$ , defined on the domain  $\{\mathbf{w} \in \mathbb{R}^{p+d} \mid \mathbf{w} = \nabla_{\mathbf{v}} \phi^*(\mathbf{v}) \text{ for some } \mathbf{v} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^d\}$ .

We compute from (24) that elements of this domain satisfy

$$\begin{aligned} w_i &= W_i^0 \exp\left(\frac{m_i}{k_B T} \left(v_i + \frac{1}{2} \mathbf{v}_{p+1}^2\right)\right) > 0, \quad 1 \leq i \leq p \\ \mathbf{w}_{p+1} &= \left(\sum_{i=1}^p W_i^0 \exp\left(\frac{m_i}{k_B T} \left(v_i + \frac{1}{2} \mathbf{v}_{p+1}^2\right)\right)\right) \mathbf{v}_{p+1} = \left(\sum_{i=1}^p w_i\right) \mathbf{v}_{p+1}. \end{aligned}$$

The same kind of computations as for  $\eta^*$  eventually lead to

$$(25) \quad \phi(\mathbf{w}) = \sum_{i=1}^p \frac{k_B T}{m_i} w_i \left[ \ln\left(\frac{w_i}{W_i^0}\right) - 1 \right] + \frac{1}{2} \frac{\mathbf{w}_{p+1}^2}{\sigma(\mathbf{w})}.$$

Then, following [4], the equilibrium function can be defined by

$$\mathcal{E}(\mathbf{w}) = \nabla_{\mathbf{v}} \eta^*(\nabla_{\mathbf{w}} \phi(\mathbf{w})^\top \mathbb{Q}).$$

Let us compute

$$\nabla_{\mathbf{w}} \phi(\mathbf{w})^\top = \left[ \frac{k_B T}{m_1} \ln\left(\frac{w_1}{W_1^0}\right) - \frac{1}{2} \left(\frac{\mathbf{w}_{p+1}}{\sigma(\mathbf{w})}\right)^2, \dots, \frac{k_B T}{m_p} \ln\left(\frac{w_p}{W_p^0}\right) - \frac{1}{2} \left(\frac{\mathbf{w}_{p+1}}{\sigma(\mathbf{w})}\right)^2, \frac{\mathbf{w}_{p+1}^\top}{\sigma(\mathbf{w})} \right].$$

Besides, observe that

$$\nabla_{\mathbf{V}} \eta^*(\mathbf{V}) = \begin{bmatrix} G^1(\mathbf{V}) \\ G^2(\mathbf{V}) \end{bmatrix},$$

where

$$\begin{aligned} G^1(\mathbf{V}) &= \left[ W_1^0 \exp\left(\frac{m_1}{k_B T} \left(V_1 + \frac{1}{2} \mathbf{V}_{p+1}^2\right)\right), \dots, W_p^0 \exp\left(\frac{m_p}{k_B T} \left(V_p + \frac{1}{2} \mathbf{V}_{2p}^2\right)\right) \right]^\top, \\ G^2(\mathbf{V}) &= \left[ W_1^0 \exp\left(\frac{m_1}{k_B T} \left(V_1 + \frac{1}{2} \mathbf{V}_{p+1}^2\right)\right) \mathbf{V}_{p+1}^\top, \dots, W_p^0 \exp\left(\frac{m_p}{k_B T} \left(V_p + \frac{1}{2} \mathbf{V}_{2p}^2\right)\right) \mathbf{V}_{2p}^\top \right]^\top. \end{aligned}$$

The result of Proposition 5 immediately follows from those computations.  $\square$

**Remark 1.** Thanks to (20), we already know that there exists  $\mathbf{u} \in \mathbb{R}^d$  such that

$$\mathcal{E}(\mathbf{w}) = [w_1, \dots, w_p, w_1 \mathbf{u}^\top, \dots, w_p \mathbf{u}^\top]^\top.$$

Hence, it is clear that  $\mathbf{u}$  and  $\mathbf{w}_{p+1}$  are connected by the relationship  $\mathbf{w}_{p+1} = \sigma(\mathbf{w}) \mathbf{u}$ . In terms of (7), that means that  $\mathcal{E}(\mathbf{w})$  writes

$$(26) \quad \mathcal{E}(\mathbf{w}) = [\rho_1, \dots, \rho_p, \rho_1 \mathbf{u}^\top, \dots, \rho_p \mathbf{u}^\top]^\top.$$

**Remark 2.** For any  $\mathbf{w} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^d$ , there holds

$$(27) \quad \mathbb{Q} \mathcal{E}(\mathbf{w}) = \mathbf{w},$$

$$(28) \quad \mathbb{Q} \nabla_{\mathbf{w}} \mathcal{E}(\mathbf{w}) = \mathbb{I}_{p+d},$$

These relations are known from the general setting [4], and can of course be checked by computations by blocks.

Relation (28) implies that for any  $\mathbf{w} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^d$ , the matrix  $\mathbb{P}(\mathbf{w}) = \nabla_{\mathbf{w}} \mathcal{E}(\mathbf{w}) \mathbb{Q} \in \mathbb{R}^{(p+d) \times (p+d)}$  is a projection onto the  $(p+d)$ -dimensional manifold of local equilibria. Its properties are stated in the following proposition.

**Proposition 6.** *For any  $\mathbf{w} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^d$ ,  $\mathbb{P}(\mathbf{w}) = \nabla_{\mathbf{w}} \mathcal{E}(\mathbf{w}) \mathbb{Q}$  is a projection matrix, that is  $\mathbb{P}(\mathbf{w})^2 = \mathbb{P}(\mathbf{w})$ . It has the form*

$$\mathbb{P}(\mathbf{w}) = \begin{bmatrix} \mathbb{I}_p & \mathbf{0}_{p \times dp} \\ \mathbb{P}_{21}(\mathbf{w}) & \mathbb{P}_{22}(\mathbf{w}) \end{bmatrix},$$

where

$$\mathbb{P}_{21}(\mathbf{w}) = \frac{1}{\sigma(\mathbf{w})^2} \begin{bmatrix} (\sigma(\mathbf{w}) - w_1) \mathbf{w}_{p+1} & -w_1 \mathbf{w}_{p+1} & \cdots & -w_1 \mathbf{w}_{p+1} \\ -w_2 \mathbf{w}_{p+1} & (\sigma(\mathbf{w}) - w_2) \mathbf{w}_{p+1} & \cdots & -w_2 \mathbf{w}_{p+1} \\ \vdots & \vdots & \ddots & \vdots \\ -w_p \mathbf{w}_{p+1} & -w_p \mathbf{w}_{p+1} & \cdots & (\sigma(\mathbf{w}) - w_p) \mathbf{w}_{p+1} \end{bmatrix} \in \mathbb{R}^{dp \times p},$$

and

$$\mathbb{P}_{22}(\mathbf{w}) = \frac{1}{\sigma(\mathbf{w})} \begin{bmatrix} w_1 \mathbb{I}_d & \cdots & w_1 \mathbb{I}_d \\ \vdots & \ddots & \vdots \\ w_p \mathbb{I}_d & \cdots & w_p \mathbb{I}_d \end{bmatrix} \in \mathbb{R}^{dp \times dp}.$$

Finally, for any  $\mathbf{w} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^d$ , the kernel of  $\mathbb{P}(\mathbf{w})$  is given by

$$\ker \mathbb{P}(\mathbf{w}) = \left\{ \mathbf{W} \in \mathbb{R}^{p+dp} \mid W_i = 0, 1 \leq i \leq p \text{ and } \sum_{i=1}^p \mathbf{W}_{p+i} = \mathbf{0} \right\}.$$

*Proof.* The fact that  $\mathbb{P}(\mathbf{w})$  is a projection is straightforward thanks to (28). Introducing

$$\mathbb{H}_{22}(\mathbf{w}) = \frac{1}{\sigma(\mathbf{w})} \begin{bmatrix} w_1 \mathbb{I}_d \\ \vdots \\ w_p \mathbb{I}_d \end{bmatrix} \in \mathbb{R}^{dp \times d},$$

we compute

$$\nabla_{\mathbf{w}} \mathcal{E}(\mathbf{w}) = \begin{bmatrix} \mathbb{I}_p & \mathbf{0}_{p \times d} \\ \mathbb{P}_{21}(\mathbf{w}) & \mathbb{H}_{22}(\mathbf{w}) \end{bmatrix},$$

and block computations lead to the required expression of  $\mathbb{P}(\mathbf{w})$ . The expression of the kernel of the operator  $\mathbb{P}(\mathbf{w})$  immediately follows.  $\square$

### 3. STUDY OF THE STIFF SYSTEM NEAR A LOCAL EQUILIBRIUM

As it is stated in [4], whenever the local equilibrium approximation is hyperbolic, it makes sense to seek a first-order correction. The conserved quantities  $\mathbf{w}$  can be used as coordinates for a subset of functions  $\mathbf{W} = \mathcal{M}[\mathbf{w}]$  with  $\mathbb{Q}\mathbf{W} = \mathbf{w}$  that is approximately invariant under the evolution (8):

$$\partial_t \mathbf{W} + \nabla \cdot (\mathbb{Q}\mathbf{F}(\mathcal{M}[\mathbf{w}])) \simeq 0.$$

Thus, since  $\mathbf{W} = \mathcal{M}[\mathbf{w}]$  satisfies (8), we have

$$(29) \quad 0 = \partial_t \mathbf{W} + \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{W}) + \frac{1}{\varepsilon} \mathbf{R}(\mathbf{W}) \simeq (\mathbb{I}_{p+dp} - \nabla_{\mathbf{w}} \mathcal{M}[\mathbf{w}] \mathbb{Q}) \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{M}[\mathbf{w}]) + \frac{1}{\varepsilon} \mathbf{R}(\mathcal{M}[\mathbf{w}]).$$

Since we consider the local equilibrium approximation, it is natural to seek a formal expansion of  $\mathbf{W}$  in powers of  $\varepsilon$  as

$$\mathbf{W}^\varepsilon = \mathcal{E}(\mathbf{w}) + \varepsilon \mathcal{M}^{(1)}[\mathbf{w}] + \cdots.$$

Linearizing the right hand side of (29) and writing order 1 in  $\varepsilon$  leads to

$$(\mathbb{I}_{p+dp} - \nabla_{\mathbf{w}} \mathcal{E}(\mathbf{w}) \mathbb{Q}) \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})) + \nabla_{\mathbf{W}} \mathbf{R}(\mathcal{E}(\mathbf{w})) \mathcal{M}^{(1)}[\mathbf{w}] = 0$$

Provided the inversion of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  is possible, this gives us the first-order correction term  $\mathcal{M}^{(1)}[\mathbf{w}]$  and the equation satisfied by the conserved quantities  $\mathbf{w}$ .

Therefore, in Section 3.1, we shall describe in a precise way the space on which the pseudo-inversion of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  is performed. Then, in Section 3.2, we shall compute explicitly the local equilibrium and its first-order correction term, which are given by the following theorem (see Chen, Levermore and Liu's computations [4, Eq. (2.23)]).

**Theorem 1.** *The first-order correction, given by*

$$\mathcal{M}^{(1)}[\mathbf{w}] = -\mathbb{B} [\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w})] \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})),$$

where  $\mathbb{B}$  denotes the pseudo-inverse of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  such that  $\text{im } \mathbb{B} = \ker \mathbb{Q}$ , is locally dissipative with respect to the entropy  $\eta$ . The reduced system reads

$$(30) \quad \partial_t \mathbf{w} + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{w}) = \varepsilon \nabla_{\mathbf{x}} \cdot \mathbf{g}(\mathbf{w}),$$

where, for any  $1 \leq k \leq d$ ,

$$\begin{aligned} \mathbf{f}_k(\mathbf{w}) &= \mathbb{Q} \mathbf{F}_k(\mathcal{E}(\mathbf{w})), \\ \mathbf{g}_k(\mathbf{w}) &= \mathbb{Q} \nabla_{\mathbf{W}} \mathbf{F}_k(\mathcal{E}(\mathbf{w})) \mathbb{B} [\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w})] \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})). \end{aligned}$$

It satisfies that the local equilibrium approximation is hyperbolic.

**3.1. Pseudo-inversion of the matrix  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$ .** As we stated, we are led to compute  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  to linearize the source term near  $\mathcal{E}(\mathbf{w})$ , and to define its pseudo-inverse.

We differentiate  $\nabla_{\mathbf{W}}\mathbf{R}(\mathbf{W})$  as follows:

$$(31) \quad \nabla_{\mathbf{W}}\mathbf{R}(\mathbf{W}) = \begin{bmatrix} \mathbf{0}_{p \times p} & \mathbf{0}_{p \times dp} \\ \mathbb{G}_{21} & \mathbb{G}_{22} \end{bmatrix},$$

where

$$\mathbb{G}_{21} = \text{Diag}_{dp \times p} \left( \sum_{j=1}^p a_{ij} \mathbf{W}_{p+j} \right), \quad \mathbb{G}_{22} = \begin{bmatrix} a_{11} W_1 \mathbb{I}_d & \cdots & a_{1p} W_1 \mathbb{I}_d \\ \vdots & & \vdots \\ a_{p1} W_p \mathbb{I}_d & \cdots & a_{pp} W_p \mathbb{I}_d \end{bmatrix}.$$

Recalling the value (26) of  $\mathcal{E}(\mathbf{w}) = [\rho_1, \dots, \rho_p, \rho_1 \mathbf{u}^\top, \dots, \rho_p \mathbf{u}^\top]^\top$ , the matrix  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  has the same structure as in (31), with

$$(32) \quad \mathbb{G}_{21} = \mathbf{0}_{dp \times p}, \quad \mathbb{G}_{22} = \begin{bmatrix} a_{11} \rho_1 \mathbb{I}_d & \cdots & a_{1p} \rho_1 \mathbb{I}_d \\ \vdots & & \vdots \\ a_{p1} \rho_p \mathbb{I}_d & \cdots & a_{pp} \rho_p \mathbb{I}_d \end{bmatrix}.$$

The following proposition sums up properties on the null space and range of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$ , which allow to define its pseudo-inverse.

**Proposition 7.** *The operator  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  satisfies, for any  $\mathbf{w} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^d$ ,*

$$(33) \quad \text{im}(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))) = \ker \mathbb{Q}.$$

Moreover, we have

$$(34) \quad \mathbb{R}^{p+dp} = \ker(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))) \oplus \text{im}(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))).$$

This allows to define  $\mathbb{B}$  the pseudo-inverse of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  with prescribed range  $\ker \mathbb{Q}$  and null space  $\ker(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w})))$ .

*Proof.* In order to compute  $\text{im}(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w})))$ , observe that for any  $\mathbf{W} \in \mathbb{R}^{p+d}$  of the form (6), a direct block computation gives

$$(35) \quad \nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))\mathbf{W} = \left[ 0, \dots, 0, \sum_{j=1}^p a_{1j}W_1\mathbf{W}_{p+j}^\top, \dots, \sum_{j=1}^p a_{pj}W_p\mathbf{W}_{p+j}^\top \right]^\top.$$

Note that  $W_i\mathbf{W}_{p+j}$  can have an arbitrary value in  $\mathbb{R}^d$  for any  $1 \leq j \leq p$ . Then, taking into account the property (3) of  $\mathbb{A}$  and the definition (19) of the null space of  $\mathbb{Q}$ , it follows

$$\text{im}(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))) = \left\{ \left[ 0, \dots, 0, \mathbf{X}_{p+1}^\top, \dots, \mathbf{X}_{2p}^\top \right]^\top, \sum_{i=1}^p \mathbf{X}_{p+i} = \mathbf{0}_{d \times 1} \right\} = \ker \mathbb{Q}.$$

It is clear that the dimension of the image of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$  is  $d(p-1)$ . To obtain (34), we determine the null space of  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$ . From (35), it is clear that the first  $p$  components of any  $\mathbf{W}$  in this null space can be arbitrary. The remaining components  $\mathbf{W}_{p+j}$  need to satisfy

$$\sum_{j=1}^p a_{ij}W_i\mathbf{W}_{p+j} = \sum_{j=1}^p \alpha_{ij} \frac{\mathbf{W}_{p+j}}{W_j} = \mathbf{0}_{d \times 1}, \quad 1 \leq i \leq p.$$

From property (3) of  $\mathbb{A}$ , and in the same way as in Proposition 3, there exists  $\mathbf{v} \in \mathbb{R}^d$  such that

$$\frac{\mathbf{W}_{p+j}}{W_j} = \mathbf{v}, \quad 1 \leq j \leq p.$$

Thus

$$\ker(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))) = \left\{ [W_1, \dots, W_p, W_1\mathbf{v}^\top, \dots, W_p\mathbf{v}^\top]^\top, \mathbf{v} \in \mathbb{R}^d, W_i \in \mathbb{R}, 1 \leq i \leq p \right\},$$

which is of dimension  $p+d$ . To conclude the proof, for  $\mathbf{W} \in \ker(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))) \cap \text{im}(\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w})))$ , there holds

$$\begin{cases} \mathbf{W} = [0, \dots, 0, \mathbf{X}_{p+1}^\top, \dots, \mathbf{X}_{2p}^\top]^\top \text{ with } \sum_i \mathbf{X}_{p+i} = \mathbf{0}_{d \times 1}, \\ \mathbf{W} = [W_1, \dots, W_p, W_1\mathbf{v}^\top, \dots, W_p\mathbf{v}^\top]^\top, \end{cases}$$

which immediately implies that  $\mathbf{W} = \mathbf{0}_{(p+d) \times 1}$ . Thanks to the rank-nullity theorem on  $\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))$ , we deduce (34). The definition of the pseudo-inverse  $\mathbb{B}$  then follows (see Proposition 10 in Appendix).  $\square$

**3.2. Local equilibrium approximation and first-order correction.** We are now in a position to compute explicitly  $\mathbf{f}_k$  and  $\mathbf{g}_k$  defined in Theorem 1. Let us first compute the left-hand side of (30).

**Proposition 8.** *The convective part of the reduced system is given by*

$$\partial_t \mathbf{w} + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{w}) = \begin{bmatrix} \partial_t \rho_1 + \nabla_{\mathbf{x}} \cdot (\rho_1 \mathbf{u}) \\ \vdots \\ \partial_t \rho_p + \nabla_{\mathbf{x}} \cdot (\rho_p \mathbf{u}) \\ \partial_t \rho \mathbf{u} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \sum_{k=1}^d \partial_{x_k} P, \end{bmatrix}$$

where  $P = \sum_i P_i(\rho_i)$ .

*Proof.* From (26), we have

$$\mathbf{F}_k(\mathcal{E}(\mathbf{w})) = [\rho_1 \mathbf{u} \cdot \mathbf{e}_k, \dots, \rho_p \mathbf{u} \cdot \mathbf{e}_k, \rho_1 \mathbf{u} \cdot \mathbf{e}_k \mathbf{u}^\top + P_1(\rho_1) \mathbf{e}_k^\top, \dots, \rho_p \mathbf{u} \cdot \mathbf{e}_k \mathbf{u}^\top + P_p(\rho_p) \mathbf{e}_k^\top]^\top.$$

When multiplying by the matrix  $\mathbb{Q}$ , we get exactly the result of the proposition.  $\square$

We shall now compute the right hand side of (30).

**Proposition 9.** *The diffusive part of the reduced system reads as*

$$\nabla_{\mathbf{x}} \cdot \mathbf{g}(\mathbf{w}) = \begin{bmatrix} \nabla_{\mathbf{x}} \cdot \left( \rho_1 \sum_{j=1}^p \lambda_{1j} \nabla_{\mathbf{x}} P_j(\rho_j) \right) \\ \vdots \\ \nabla_{\mathbf{x}} \cdot \left( \rho_p \sum_{j=1}^p \lambda_{pj} \nabla_{\mathbf{x}} P_j(\rho_j) \right) \\ \mathbf{0}_{d \times 1} \end{bmatrix},$$

where  $\mathbb{L} = (\lambda_{ij})_{1 \leq i, j \leq p}$  is the unique pseudo-inverse of the Maxwell-Stefan matrix  $\mathbb{A}$  with prescribed range  $(\text{Span } \mathbf{r})^\perp$  and null space  $\text{Span } \mathbf{r}$ , with  $\mathbf{r} = [\rho_1, \dots, \rho_p]^\top$ . The matrix  $\mathbb{L}$  is symmetric non-positive. Moreover,  $\mathbb{L}$  has the form  $\left( \frac{1}{W_i W_j} \ell_{ij} \right)_{1 \leq i, j \leq p}$ , where the coefficients  $(\ell_{ij})$  do not depend on  $\mathbf{W}$ .

*Proof.* We compute

$$\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})) = \begin{bmatrix} \nabla_{\mathbf{x}} \cdot \left( \frac{w_1}{\sigma(\mathbf{w})} \mathbf{w}_{p+1} \right) \\ \vdots \\ \nabla_{\mathbf{x}} \cdot \left( \frac{w_p}{\sigma(\mathbf{w})} \mathbf{w}_{p+1} \right) \\ \nabla_{\mathbf{x}} \cdot \left( \frac{w_1}{\sigma(\mathbf{w})^2} \mathbf{w}_{p+1} \otimes \mathbf{w}_{p+1} \right) + \nabla_{\mathbf{x}} P_1(w_1) \\ \vdots \\ \nabla_{\mathbf{x}} \cdot \left( \frac{w_p}{\sigma(\mathbf{w})^2} \mathbf{w}_{p+1} \otimes \mathbf{w}_{p+1} \right) + \nabla_{\mathbf{x}} P_p(w_p) \end{bmatrix},$$

and

$$\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w}) = \begin{bmatrix} \mathbf{0}_{p \times p} & \mathbf{0}_{p \times dp} \\ -\mathbb{P}_{21}(\mathbf{w}) & \mathbb{I}_{dp} - \mathbb{P}_{22}(\mathbf{w}) \end{bmatrix}.$$

We are now in the position to compute the product  $(\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w})) \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w}))$ . Nevertheless, for a better understanding, we switch to the classical notations (7) of  $\mathbf{w}$  in terms of  $\rho_i$  and  $\mathbf{u}$ . Hence, we can write

$$\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})) = \begin{bmatrix} \nabla_{\mathbf{x}} \cdot (\rho_1 \mathbf{u}) \\ \vdots \\ \nabla_{\mathbf{x}} \cdot (\rho_p \mathbf{u}) \\ \nabla_{\mathbf{x}} \cdot (\rho_1 \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} P_1(\rho_1) \\ \vdots \\ \nabla_{\mathbf{x}} \cdot (\rho_p \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} P_p(\rho_p) \end{bmatrix},$$

and, defining  $\rho = \sum \rho_i$ ,

$$\mathbb{P}_{21}(\mathbf{w}) = \frac{1}{\rho} \begin{bmatrix} (\rho - \rho_1) \mathbf{u} & -\rho_1 \mathbf{u} & \cdots & -\rho_1 \mathbf{u} \\ -\rho_2 \mathbf{u} & (\rho - \rho_2) \mathbf{u} & \cdots & -\rho_2 \mathbf{u} \\ \vdots & \vdots & \ddots & \vdots \\ -\rho_p \mathbf{u} & -\rho_p \mathbf{u} & \cdots & (\rho - \rho_p) \mathbf{u} \end{bmatrix}, \quad \mathbb{P}_{22}(\mathbf{w}) = \frac{1}{\rho} \begin{bmatrix} \rho_1 \mathbb{I}_d & \cdots & \rho_1 \mathbb{I}_d \\ \vdots & \ddots & \vdots \\ \rho_p \mathbb{I}_d & \cdots & \rho_p \mathbb{I}_d \end{bmatrix}.$$

If we compute the rows  $p+1, \dots, p+d$  of  $(\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w}))\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w}))$ , we obtain the following vector

$$-\mathbf{u}\nabla_{\mathbf{x}} \cdot (\rho_1\mathbf{u}) + \frac{\rho_1}{\rho}\mathbf{u}\nabla_{\mathbf{x}} \cdot (\rho\mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho_1\mathbf{u} \otimes \mathbf{u}) - \frac{\rho_1}{\rho}\nabla_{\mathbf{x}} \cdot (\rho\mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}}P_1(\rho_1) - \frac{\rho_1}{\rho} \sum_{j=1}^p P_j(\rho_j),$$

which simplifies into

$$\nabla_{\mathbf{x}}P_1(\rho_1) - \frac{\rho_1}{\rho}\nabla_{\mathbf{x}}P,$$

where  $P = \sum_j P_j(\rho_j)$ . The following rows are computed in the same way. Therefore,

$$(\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w}))\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})) = \begin{bmatrix} 0_{p \times 1} \\ \nabla_{\mathbf{x}}P_1(\rho_1) - \frac{\rho_1}{\rho}\nabla_{\mathbf{x}}P \\ \vdots \\ \nabla_{\mathbf{x}}P_p(\rho_p) - \frac{\rho_p}{\rho}\nabla_{\mathbf{x}}P \end{bmatrix}.$$

We want to compute  $\mathbf{W} = \mathbb{B}(\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w}))\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w}))$ . Since  $\mathbf{W} \in \text{im } \mathbb{B} = \text{ker } \mathbb{Q}$ , it immediately follows that  $W_i = 0$ ,  $1 \leq i \leq p$  and  $\sum_j \mathbf{W}_{p+j} = 0$ . Besides, it is clear that

$$(\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w}))\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})) \in \text{ker } \mathbb{Q} = \text{im } \nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w})).$$

Thanks to Corollary 1, we can state that

$$\nabla_{\mathbf{W}}\mathbf{R}(\mathcal{E}(\mathbf{w}))\mathbf{W} = (\mathbb{I}_{p+dp} - \mathbb{P}(\mathbf{w}))\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathcal{E}(\mathbf{w})).$$

Using (35), this implies, for any  $1 \leq i \leq p$ ,

$$\sum_{j=1}^p \frac{\alpha_{ij}}{\rho_j} \mathbf{W}_{p+j} = \nabla_{\mathbf{x}}P_i(\rho_i) - \frac{\rho_i}{\rho}\nabla_{\mathbf{x}}P.$$

We recall that  $\text{ker } \mathbb{A} = \text{Span } \mathbf{1}_{p \times 1}$  and, by self-adjointness of  $\mathbb{A}$ ,  $\text{im } \mathbb{A} = (\text{Span } \mathbf{1}_{p \times 1})^\perp$ . Since both vectors  $\mathbf{r} = [\rho_1, \dots, \rho_p]^\top$  and  $\mathbf{1}_{p \times 1}$  are obviously not orthogonal, the decompositions

$$\mathbb{R}^p = (\text{Span } \mathbf{1}_{p \times 1}) \oplus (\text{Span } \mathbf{r})^\perp = (\text{Span } \mathbf{1}_{p \times 1})^\perp \oplus (\text{Span } \mathbf{r})$$

allow to state the existence of a unique pseudo-inverse  $\mathbb{L} = (\lambda_{ij})_{1 \leq i, j \leq p}$  of  $\mathbb{A}$  with prescribed range  $(\text{Span } \mathbf{r})^\perp$  and null space  $\text{Span } \mathbf{r}$ . Furthermore,  $\mathbb{L}$  is symmetric and non-positive. The symmetry property holds thanks to Corollary 2. The non-positivity of  $\mathbb{L}$  is a direct consequence of Corollary 1. Indeed, denoting by  $\langle \cdot, \cdot \rangle$  the scalar product on  $\mathbb{R}^p$ , we first write  $\mathbf{Z} \in \mathbb{R}^p$  as the sum of  $\mathbf{Y} \in (\text{Span } \mathbf{1}_{p \times 1})^\perp = \text{im } \mathbb{A}$  and  $\gamma\mathbf{r}$ ,  $\gamma \in \mathbb{R}$ . From the orthogonality of  $\mathbf{Y}$  and  $\mathbf{r}$  and the fact that  $\mathbf{r} \in \text{ker } \mathbb{L}$ , we have

$$\langle \mathbb{L}\mathbf{Z}, \mathbf{Z} \rangle = \langle \mathbb{L}\mathbf{Y}, \mathbf{Y} \rangle = \langle \mathbf{X}, \mathbb{A}\mathbf{X} \rangle \leq 0,$$

where  $\mathbf{X} = \mathbb{L}\mathbf{Y}$  is the only element of  $\text{im } \mathbb{L} = (\text{Span } \mathbf{r})^\perp$  such that  $\mathbb{A}\mathbf{X} = \mathbf{Y}$ .

Then we can write for any  $1 \leq i \leq p$ , thanks to Corollary 1,

$$\mathbf{W}_{p+i} = \rho_i \sum_{j=1}^p \lambda_{ij} \left( \nabla_{\mathbf{x}}(P_j(\rho_j)) - \frac{\rho_j}{\rho}\nabla_{\mathbf{x}}P \right).$$

Since  $\mathbf{r}$  spans  $\text{ker } \mathbb{L}$ , *i.e.* for any  $1 \leq i \leq p$ ,  $\sum_j \lambda_{ij}\rho_j = 0$ , the previous equality becomes

$$\mathbf{W}_{p+i} = \rho_i \sum_{j=1}^p \lambda_{ij} \nabla_{\mathbf{x}}(P_j(\rho_j)).$$

Now we compute the remaining part of the right-hand side. From (17) and (26), we know that

$$\nabla_{\mathbf{W}} \mathbf{F}_k(\mathcal{E}(\mathbf{w})) = \begin{bmatrix} \mathbf{0}_{p \times p} & \text{Diag}_{p \times dp}(\mathbf{e}_k^\top) \\ \text{Diag}_{dp \times p}(-(\mathbf{u} \cdot \mathbf{e}_k)\mathbf{u} + P'_i(\rho_i)\mathbf{e}_k) & \text{Diag}_{dp \times dp}((\mathbf{u} \cdot \mathbf{e}_k)\mathbb{I}_d + \mathbf{u} \otimes \mathbf{e}_k) \end{bmatrix}.$$

We then get

$$\mathbb{Q} \nabla_{\mathbf{W}} \mathbf{F}_k(\mathcal{E}(\mathbf{w})) = \begin{bmatrix} \mathbf{0}_{p \times p} & \text{Diag}_{p \times dp}(\mathbf{e}_k^\top) \\ \mathbb{M}_{21} & \mathbb{M}_{22} \end{bmatrix} \in \mathbb{R}^{(p+d) \times (p+dp)},$$

where

$$\mathbb{M}_{21} = [-(\mathbf{u} \cdot \mathbf{e}_k)\mathbf{u} + P'_1(\rho_1)\mathbf{e}_k, \dots, -(\mathbf{u} \cdot \mathbf{e}_k)\mathbf{u} + P'_p(\rho_p)\mathbf{e}_k] \in \mathbb{R}^{d \times p},$$

$$\mathbb{M}_{22} = [(\mathbf{u} \cdot \mathbf{e}_k)\mathbb{I}_d + \mathbf{u} \otimes \mathbf{e}_k, \dots, (\mathbf{u} \cdot \mathbf{e}_k)\mathbb{I}_d + \mathbf{u} \otimes \mathbf{e}_k] \in \mathbb{R}^{d \times dp}.$$

Block computations lead to

$$\mathbf{g}_k(\mathbf{w}) = \mathbb{Q} \nabla_{\mathbf{W}} \mathbf{F}_k(\mathcal{E}(\mathbf{w})) \mathbf{W} = \begin{bmatrix} \mathbf{W}_{p+1} \cdot \mathbf{e}_k \\ \vdots \\ \mathbf{W}_{2p} \cdot \mathbf{e}_k \\ (\mathbf{u} \cdot \mathbf{e}_k) \sum_{i=1}^p \mathbf{W}_{p+i} + \sum_{i=1}^p (\mathbf{W}_{p+i} \cdot \mathbf{e}_k) \mathbf{u} \end{bmatrix}.$$

Using the fact that  $\sum_i \mathbf{W}_{p+i} = \mathbf{0}$ , we deduce

$$\mathbf{g}_k(\mathbf{w}) = \begin{bmatrix} \rho_1 \sum_{j=1}^p \lambda_{1j} \partial_{x_k} P_j(\rho_j) \\ \vdots \\ \rho_p \sum_{j=1}^p \lambda_{pj} \partial_{x_k} P_j(\rho_j) \\ \mathbf{0}_{d \times 1} \end{bmatrix}.$$

Finally, let us check that  $\mathbb{L}$  has the form  $\left(\frac{1}{\rho_i \rho_j} \ell_{ij}\right)_{1 \leq i, j \leq p}$ , where the coefficients  $(\ell_{ij})$  do not depend on  $\mathbf{W}$ . Indeed, one can introduce  $\hat{\mathbb{A}} = (a_{ij})$ , which does not depend either on  $\mathbf{W}$ . Denoting by  $\Delta = \text{Diag}_{p \times p}(W_i)$ , we can write  $\mathbb{A} = \Delta \hat{\mathbb{A}} \Delta$ . Let us set  $\hat{\mathbb{L}} = \Delta \mathbb{L} \Delta$ . It is clear that  $\hat{\mathbb{L}}$  is the pseudo-inverse of  $\hat{\mathbb{A}}$  with prescribed range  $(\text{Span } \mathbf{1}_{p \times 1})^\perp$  and null space  $\text{Span } \mathbf{1}_{p \times 1}$ , and consequently does not depend on  $\mathbf{W}$ . Then  $\mathbb{L} = \Delta^{-1} \hat{\mathbb{L}} \Delta^{-1}$  has the expected form.  $\square$

#### APPENDIX A. ADDENDUM ON PSEUDO-INVERSES

In order to help the reader if necessary, we briefly recall some results on pseudo-inverses which are used in the article. The first one allows to define pseudo-inverse matrices, it is a classical property which can be found, for instance, in [5, Prop. 7.3.5, p. 164].

**Proposition 10.** *Let  $\mathbb{A} \in \mathbb{R}^{p \times p}$  with null space  $\ker \mathbb{A}$  and range  $\text{im } \mathbb{A}$ . Let  $S$  and  $T$  be two subspaces of  $\mathbb{R}^p$  such that  $\mathbb{R}^p = \ker \mathbb{A} \oplus S$  and  $\mathbb{R}^p = \text{im } \mathbb{A} \oplus T$ . Then there exists a unique matrix  $\mathbb{B}$  such that:*

- (1)  $\mathbb{A} \mathbb{B} \mathbb{A} = \mathbb{A}$ ,
- (2)  $\mathbb{B} \mathbb{A} \mathbb{B} = \mathbb{B}$ ,
- (3)  $\ker \mathbb{B} = T$  and  $\text{im } \mathbb{B} = S$ .

This matrix  $\mathbb{B}$  is then called the pseudo-inverse of  $\mathbb{A}$  with prescribed range  $S$  and null space  $T$ .

As a consequence of the previous proposition defining the pseudo-inverse of a matrix with prescribed range and null space, the following corollary justifies the “inverse” name.

**Corollary 1.** *Let  $\mathbb{B}$  be the pseudo-inverse of  $\mathbb{A}$  with prescribed range  $\text{im } \mathbb{B}$  and null space  $\ker \mathbb{B}$ . Let  $Y \in \text{im } \mathbb{A}$ . Then there exists a unique  $X \in \text{im } \mathbb{B}$  such that  $\mathbb{A}X = Y$ , it is given by  $X = \mathbb{B}Y$ .*

The previous corollary is supplemented with the following one, which focuses on the symmetric case.

**Corollary 2.** *Consider a symmetric matrix  $\mathbb{A} \in \mathbb{R}^{p \times p}$ , and a subspace  $T$  such that  $\mathbb{R}^p = \text{im } \mathbb{A} \oplus T$ . Then the only symmetric pseudo-inverse of  $\mathbb{A}$  is the one with prescribed range  $T^\perp$  and null space  $T$ .*

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