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# Development of a Relaxation Scheme for Weakly Ionised Gases

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#### Nomenclature

a	Relaxation parameter
c	Sound speed
$C_{v,t}$	Specific heat at constant volume
	for the translation mode
$C_{v,t}^i$	Specific heat at constant volume
v, v	for the translation mode of the i-th species
$e_v$	Vibrational energy
Ē	Total energy of the mixture
$E_e$	Total energy of the electron gas
ε	Electric field
$h^0$	Heat of formation
$\mathcal{M}_e$	Molar mass of the electron
$\mathcal{M}_i$	Molar mass of the i-th species
p	Pressure of the heavy species
$p_e$	Pressure of the electron gas
$q_e$	Electron charge
${\cal R}$	Universal gas constant
$S_e$	Entropy of the electron gas
T	Temperature
$T_e$	Electron temperature
u	Velocity
$Y_e$	Mass fraction of the electrons
$Y_i$	Mass fraction of the i-th species
$\gamma$	Polytropic coefficient
$ ho_e$	Electron density $(\rho_e = \rho Y_e)$
$ ho_i$	Density of the i-th species $(\rho_i = \rho Y_i)$
ho	Density $(\rho = \rho_e + \sum \rho_i)$
au	Inverse of the density

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#### Subscripts

e Electron

*i* Heavy species

*j* Molecular species

### Introduction

This work treats the numerical approximation of the convective diffusive system governing ionized mixtures of reacting gases in thermal nonequilibrium. Such plasmas are studied here in the context of large Mach number flows corresponding to hypersonic flows At high speeds, the flow around reentry bodies. reaches extremely high temperatures near the vehicle. These temperatures are high enough to induce vibrational excitation, dissociation of diatomic molecules and ionization. For a better description of the flow, it is necessary to introduce different temperatures, that are another way to express the value of energy. Whereas it is a good assumption to take translational and rotational modes of heavy species in thermal equilibrium, vibrational modes of polyatomic molecules and translational mode of electron gas have to be characterized by their own temperatures.

Many different workers have performed simulations<sup>1–5</sup> of such weakly ionized flows, using the governing equations proposed by Appleton-Bray<sup>6</sup> and Lee<sup>7</sup>. These approaches have been derived for gas mixtures containing electrons, neutral and ionized species, the ions being singly-ionized and positively charged. Note that the corresponding system is naturally written in a non-conservative form due to the work of the electric field  $\mathcal{E}$ .

Basically, we can write the associated system in short form as

$$\partial_t \mathbf{u} + \mathcal{A}(\mathbf{u}) \partial_x \mathbf{u} - \partial_x (\mathcal{D}(\mathbf{u}) \partial_x \mathbf{u}) = \omega(\mathbf{u}), \quad (1)$$
  
with  $t > 0, \ x \in \mathbb{R}.$ 

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where the last two terms of the left-hand side represent respectively the convective and the diffusive effects while  $\omega(\mathbf{u})$  is a source term. In the paper, we will focus on the numerical approximation of the underlying first order system

$$\partial_t \mathbf{u} + \mathcal{A}(\mathbf{u})\partial_x \mathbf{u} = 0, \quad \text{with} \quad t > 0, \ x \in \mathbb{R},$$
 (2)

which constitutes an essential step in the treatment of the full system (1).

As the nonlinear system (2) is seen to be hyperbolic over a phase space to be precised, discontinuous solutions may occur in finite time. Thus, a major difficulty arises in that case since there does not exist a flux function **f**, such that  $\mathcal{A}(\mathbf{u}) = \nabla_{\mathbf{u}} \mathbf{f}(\mathbf{u})$ . Put in other words, system (2) is actually under a non-conservative form and the standard theory of weak solutions does apply no longer. Generally speaking, such a feature is known to make the numerical approximation of the corresponding solutions very challenging.<sup>8</sup> To overcome the problem, Coquel and Marmignon <sup>?,12</sup> have proposed to build a system of conservation laws equivalent to system (1) but under a conservative form, using specific modelling assumptions. The numerical approximation of the first-order extracted system no longer raises questions and the use of classical numerical methods becomes straightforward. To assess the relevancy of their work, they have also derived an exact Roe-type linearization.<sup>?,?,?</sup> Such an extension is not evident since the weakly ionized flow equations contain two pressures relative to the heavy species and the electron gas.

In the paper, we aim at developing a relaxation procedure for the equivalent governing equations derived by Coquel-Marmignon. In fact, this strategy presents several advantages. Let us quote, for instance, that our relaxation scheme is entropic conversely to the Roe scheme which uses numerical entropy corrections. Besides, the two inherent pressures attached to the system turn out to be very easy to manage in this context. Assessment of the relaxation scheme is performed with shocktube computations, comparing the present results with those obtained from an exact Godunov solver and the Roe-linearization proposed by Coquel-Marmignon.

### Governing equations and physical modelling

#### Non conservative system

We consider a mixture of gases made of electrons and n heavy species, ni,  $1 \leq ni \leq n$  of them being ionized. All the heavy species are described using the same velocity u. We associate a temperature T for the translational-rotational modes. Moreover,  $n\nu$ ,  $1 \leq n\nu \leq n$ , molecular species have their own vibrational temperature  $T_{v,j}$ ,  $j \in \{1, ..., n\nu\}$ . Concerning the electron gas, one defines a temperature  $T_e$  distinct from the temperature T of the heavy species mixture in order to account for the smallness of the mass ratios  $\mathcal{M}_e/\mathcal{M}_i \ll 1$ ,  $i \in \{1, ..., n\}$ . Besides, local charge neutrality is assumed.

The governing equations of the first order convective system are :

$$\begin{aligned} \partial_t(\rho Y_i) &+ \partial_x(\rho Y_i u) = 0, \quad i = 1, ..., n, \\ \partial_t(\rho u) &+ \partial_x(\rho u^2 + p + p_e) = 0, \\ \partial_t(\rho E) &+ \partial_x(\rho E + p + p_e) u = 0, \\ \partial_t(\rho Y_e E_e) &+ \partial_x(\rho Y_e E_e + p_e) u = N_e q_e \mathcal{E} u, \\ \partial_t(\rho Y_j e_{v,j}) &+ \partial_x(\rho Y_j e_{v,j} u) = 0, \quad j = 1, ..., n\nu. \end{aligned}$$

The first *n* equations represent the mass conservation of each heavy species. The next two govern respectively the conservation of the momentum  $\rho u$  and the total energy  $\rho E$  of the mixture. The last  $n\nu$  equations refer to the conservation of the vibrational energies  $\rho Y_{j}e_{v,j}$  of the  $n\nu$  molecular species that are in thermal nonequilibrium. These (n + nv + 2) conservation laws are supplemented with a balance equation : the expected conservation law for the electron gas energy  $\rho Y_e E_e$  balanced by the work of the electric field  $\mathcal{E}$ . The assumption of local charge neutrality yields the electric field  $\mathcal{E}$  from the electron gas momentum equation

$$N_e q_e \mathcal{E} = \partial_x p_e + \left\{ \partial_t (\rho Y_e u) + \partial_x (\rho Y_e u^2) \right\}.$$
(4)

The second term in the right hand side of (4) is traditionally neglected, considering the smallness of  $Y_e$  $(\mathcal{M}_e/\mathcal{M}_i << 1)$ . But in the present work, this term is kept and leads, for smooth solutions, to the following equivalent system :

$$\begin{aligned} \partial_t(\rho Y_i) &+ \partial_x(\rho Y_i u) = 0, \quad i = 1, ..., n, \\ \partial_t(\rho u) &+ \partial_x(\rho u^2 + p + p_e) = 0, \\ \partial_t(\rho E) &+ \partial_x(\rho E + p + p_e)u = 0, \end{aligned} \tag{5} \\ \partial_t(\rho Y_e E_e) &+ \partial_x(\rho Y_e E_e + p_e)u \\ &- u \partial_x p_e + Y_e u \partial_x(p + p_e) = 0, \\ \partial_t(\rho Y_j e_{v,j}) &+ \partial_x(\rho Y_j e_{v,j} u) = 0, \quad j = 1, ..., n\nu. \end{aligned}$$

Note that this system will be seen to be hyperbolic and that it is naturally written under a non conservative form as

$$\partial_t \mathbf{u} + \mathcal{A}(\mathbf{u}) \partial_x \mathbf{u} = 0, \tag{6}$$

where  $\mathbf{u}$  and  $\mathcal{A}$  find natural definitions. At the end of this section, we will derive an equivalent system of conservation laws that will be more convenient to deal with from a numerical point of view.

#### Closure relations

In this part, we present the required additional closure relations for the system under study.

We first specify the heavy species and the electron pressures. The latter one obeys the following relation

$$p_e = \kappa_e (\rho_e E_e - \frac{1}{2}\rho_e u^2), \quad \kappa_e = (\gamma_e - 1) = \frac{2}{3}, \quad (7)$$

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while the pressure law p for the mixture of heavy species is defined by

$$p = \kappa \Big( \rho E - \frac{1}{2} \rho u^2 - \frac{p_e}{\kappa_e} - \sum_{j=1}^{n\nu} \rho_j e_{v,j} - \sum_{i=1}^n \rho_i (e_i(T) + h_i^0) \Big).$$
(8)

The terms  $e_i(T)$  and  $h_i^0$  refer respectively to the energy of the internal modes at thermal equilibrium with the translational mode and to the heat of formation of the i-th species.

As each partial pressure is assumed to obey the perfect gas assumption, one defines the temperatures T and  $T_e$  by :

$$p = \rho \frac{\mathcal{R}}{\mathcal{M}} T, \quad p_e = \rho_e \frac{\mathcal{R}}{\mathcal{M}_e} T_e,$$

where the molar mass  $\mathcal{M}$  of the mixture is given by Dalton's law :

$$\frac{1}{\mathcal{M}} = \sum_{i=1}^{n} \frac{Y_i}{\mathcal{M}_i}.$$

The last term to be defined in equation (8) is the coefficient  $\kappa$  :

$$\kappa = (\gamma - 1) = \frac{\mathcal{R} \sum_{i=1}^{n} \frac{Y_i}{\mathcal{M}_i}}{C_{v,t}} = \frac{\mathcal{R}/\mathcal{M}}{C_{v,t}},$$

with

$$C_{v,t} = \sum_{i=1}^{n} Y_i C_{v,t}^i.$$

Finally, we have assumed that the flow is locally electrically neutral. The corresponding relation is :

$$\rho_e = \rho Y_e = \sum_{j=1}^{ni} \frac{\mathcal{M}_e}{\mathcal{M}_j} \rho_j. \tag{9}$$

#### Associated Conservative system

In this paper, we are interested in the numerical approximation of system (6). Since this nonlinear system is hyperbolic, its solutions are known to develop, generally speaking, discontinuities in a finite time. Thus, these solutions have to be understood as weak solutions. In this context, a major difficulty arises since the system is under a non-conservative form. Indeed, it is known that the non-conservative products involved in  $\mathcal{A}(\mathbf{u})\partial_x\mathbf{u}$  have no classical sense at the location of a shock since they cannot be given a unique definition within the standard framework of distributions. For this reason, additional informations are required in order to specify the value of the non conservative product  $\mathcal{A}(\mathbf{u})\partial_x \mathbf{u}$  at shocks. A closure equation for defining the shock solutions is therefore needed and its mathematical definition must match the underlying physics. Let us recall that system (6) comes from a more complex system :

$$\partial_t \mathbf{u} + \mathcal{A}(\mathbf{u}) \partial_x \mathbf{u} - \partial_x (\mathcal{D}(\mathbf{u}) \partial_x \mathbf{u}) = 0.$$
(10)

where the term  $\mathcal{D}$  represents the diffusive tensor including viscous, conductive and diffusive effects. The key point is that the definition of shock solutions heavily depends on the shape of the diffusive tensor  $\mathcal{D}(\mathbf{u})$ . This feature is very classical when dealing with system in non-conservative form<sup>9-11</sup>.

Once the discontinuous solutions of the nonconservative hyperbolic system (6) are defined, the system becomes well-posed and its numerical approximation could be tackled. However, using classical methods straightforwardly may lead to significant errors between the numerical and the exact solutions<sup>?, 11–13</sup> due to the non-conservative form.

To overcome these difficulties, the study of the existence of a conservative formulation for system (6) that is *compatible* with the diffusive tensor  $\mathcal{D}$  has been made by Coquel-Marmignon<sup>12</sup>. Assuming that the viscosity and the conductivity of the electrons are neglectible, they have found an equivalent convective-diffusive system under a conservative form, of which the associated first order system is

$$\begin{aligned} \partial_t \rho_i + \partial_x (\rho_i u) &= 0, \quad i = 1, \dots, n, \\ \partial_t (\rho u) + \partial_x (\rho u^2 + p + p_e) &= 0, \\ \partial_t (\rho E) + \partial_x (\rho E + p + p_e) u &= 0, \\ \partial_t (\rho S_e) + \partial_x (\rho S_e u) &= 0, \\ \partial_t (\rho_j e_{v,j}) + \partial_x (\rho_j e_{v,j} u) &= 0, \quad j = 1, \dots, n\nu, \end{aligned}$$

or equivalently

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) = 0, \tag{12}$$

with a little abuse in notation since, from now on, **u** denotes the vector  $(\{\rho_i\}_i, \rho u, \rho E, \rho S_e, \{\rho_j e_{v,j}\}_j)$  instead of  $(\{\rho_i\}_i, \rho u, \rho E, \rho Y_e E_e, \{\rho_j e_{v,j}\}_j)$ . Compared to system (5), the variable  $\rho Y_e E_e$  has been replaced by the entropy  $S_e$  of the electron gas. In this paper, we set  $S_e = p_e / \rho^{\gamma_e}$  and refer to Coquel-Marmignon<sup>12</sup> for other definitions. Considering the phase space  $\Omega \subset \mathbb{R}^N$ with  $N = n + n\nu + 3$  where

$$\Omega = \{ \mathbf{u} = {}^{T}(\{\rho_i\}_i, \rho u, \rho E, \rho S_e, \{\rho_j e_{v,j}\}_j), \\ \rho_i > 0, u \in \mathbb{R}, p(\mathbf{u}) > 0, e_{v,j} > 0, S_e > 0 \},$$

the next proposition summarizes some important properties of system (12).

**Proposition 1** The first order system is hyperbolic over  $\Omega$  and admits the following three distinct eigenvalues :

$$u - c < u < u + c,$$

where the sound speed c is defined by

$$c^{2} = \frac{\gamma_{e} p_{e} + \bar{\gamma} p}{\rho} \quad with \quad \bar{\gamma} = 1 + \frac{\mathcal{R}/\mathcal{M}}{C_{v,t} + \sum \frac{de_{i}}{dT} Y_{i}}$$

and the eigenvalue u has  $(n + n\nu + 1)$  order of multiplicity. Moreover, eigenvalues u - c and u + c are associated with genuinely non linear fields, while u is associated with linearly degenerate fields.

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Let us mention that weak solutions of system (12) are naturally selected by an entropy inequality of the form

$$\partial_t \rho S(\mathbf{u}) + \partial_x \rho S(\mathbf{u}) u \le 0, \tag{13}$$

where  $\mathbf{u} \to \rho S(\mathbf{u})$  represents a convex function. Assessment of the system for weakly ionized flows has been finally considered by developing an adapted Roe-linearization scheme. Due to the presence of the electron pressure, the extension of the Roe scheme to weakly ionized gases is not at all straightforward. However that may be, numerical simulations on realistic configurations (RAM-C) have demonstrated the interest of this approach<sup>5</sup>.

#### A relaxation model

In this section, we propose a relaxation system for approximating the weak solutions of (12). Motivated by pioneering works<sup>14–16</sup> or more recently<sup>13,17</sup>, our aim is to overcome the strong nonlinearities that make difficult the resolution of system (12). Keeping this in mind, we introduce the following non linear first order system with singular perturbation :

$$\begin{aligned} \partial_t \rho_i + \partial_x (\rho_i u) &= 0, \quad i = 1, ..., n, \\ \partial_t (\rho u) + \partial_x (\rho u^2 + \Pi) &= 0, \\ \partial_t (\rho E) + \partial_x (\rho E + \Pi) u &= 0, \\ \partial_t (\rho S_e) + \partial_x (\rho S_e u) &= 0, \\ \partial_t (\rho_j e_{v,j}) + \partial_x (\rho_j e_{v,j} u) &= 0, \quad j = 1, ..., n\nu, \\ \partial_t (\rho \Pi) + \partial_x (\rho \Pi + a^2) u &= \lambda \rho (p + p_e - \Pi), \end{aligned}$$
(14)

where solely the nonlinearities in  $p + p_e$  have been relaxed. From this definition, we observe (at least formally) that relaxation variable  $\Pi$  tends to  $p + p_e$  as  $\lambda$  goes to infinity, so that the equilibrium system (12) is recovered when the relaxation parameter  $\lambda$  tends towards that limit. In system (14), a > 0 denotes a free parameter in the relaxation procedure we propose. In the description of the numerical strategy associated with system (14), we will precise the sub-characteristic condition that the parameter a must satisfy for stability requirements.

To avoid cumbersome notations, we give system (14) the following abstract form :

$$\partial_t \mathbf{v} + \partial_x \mathcal{F}(\mathbf{v}) = \lambda \mathcal{R}(\mathbf{v}), \tag{15}$$

where both the flux  $\mathcal{F}$  and the source term  $\mathcal{R}$  find natural definitions. The phase space  $\Omega_{\mathbf{v}} \subset \mathbb{R}^{N+1}$  (recall that  $N = n + n\nu + 3$ ) for (15) is given by :

$$\Omega_{\mathbf{v}} = \{ \mathbf{v} = {}^{T}(\{\rho_i\}_i, \rho u, \rho E, \rho S_e, \{\rho_j e_{v,j}\}_j, \rho \Pi) \\ \rho_i > 0, u \in \mathbb{R}, p(\mathbf{v}) > 0, S_e > 0, e_{v,j} > 0 \}.$$

We now state the first result of this section, of which the proof is left to the reader. It proves the relevance of the relaxation model (15).

#### **Proposition 2**

Assume that a > 0. Then, the first order system extracted from (15) is hyperbolic over  $\Omega_{\mathbf{v}}$  and admits the following three real and distinct eigenvalues :

$$\lambda_{1,3}(\mathbf{v}) = u \mp a\tau = u \mp \frac{a}{\rho}, \quad \lambda_2(\mathbf{v}) = u,$$

with an order of multiplicity (N-1) for  $\lambda_2(\mathbf{v})$ . Moreover, each eigenvalue is associated with a linearly degenerate field.

The theorem makes the solution of the Riemann problem associated with (15) (when  $\lambda$  is taken to be 0) explicitly known. Since each field is linearly degenerate, the solution is indeed systematically made of four constant states, called  $\mathbf{v}_L$ ,  $\mathbf{v}_L^*$ ,  $\mathbf{v}_R^*$  and  $\mathbf{v}_R$ , separated by three contact discontinuities propagating with the characteristic speeds

$$\lambda(\mathbf{v}_L,\mathbf{v}_L^*) < \lambda(\mathbf{v}_L^*,\mathbf{v}_R^*) < \lambda(\mathbf{v}_R^*,\mathbf{v}_R),$$

where we have used clear notations. More precisely, let us recall that we necessarily have  $\lambda(\mathbf{v}_L, \mathbf{v}_L^*) = \lambda_1(\mathbf{v}_L) = \lambda_1(\mathbf{v}_L^*), \ \lambda(\mathbf{v}_L^*, \mathbf{v}_R^*) = \lambda_2(\mathbf{v}_L^*) = \lambda_2(\mathbf{v}_R^*)$ and  $\lambda(\mathbf{v}_R^*, \mathbf{v}_R) = \lambda_3(\mathbf{v}_R^*) = \lambda_3(\mathbf{v}_R)$  and that there is no entropy dissipation across contact discontinuities. Therefore, invoking the Rankine-Hugoniot jump relations across admissible discontinuities leads to the next theorem.

#### Theorem 1

Let be given  $\mathbf{v}_L$  and  $\mathbf{v}_R$  two constant states in  $\Omega_{\mathbf{v}}$ . Assume that the parameter a > 0 satisfies the condition

$$\lambda_1(\mathbf{v}_L) = u_L - a\tau_L < u^* < \lambda_3(\mathbf{v}_R) = u_R + a\tau_R,$$
$$u^* = \frac{1}{2}(u_L + u_R) + \frac{1}{2a}(\Pi_L - \Pi_R),$$
(16)

with the definition  $\tau = 1/\rho$ .

Then, the self-similar solution  $\mathbf{v}_a(x,t;\mathbf{v}_L,\mathbf{v}_R) \equiv \mathbf{v}_a(x/t;\mathbf{v}_L,\mathbf{v}_R)$  of the Cauchy problem (15) with  $\lambda = 0$  and for the initial data

$$\mathbf{v}_0(x) = \begin{cases} \mathbf{v}_L & \text{if } x < 0, \\ \mathbf{v}_R & \text{if } x > 0, \end{cases}$$
(17)

at time t = 0 is made of four constant states separated by three contact discontinuities as follows :

$$\mathbf{v}_a(x/t;\mathbf{v}_L,\mathbf{v}_R) = \begin{cases} \mathbf{v}_L & \text{if } \frac{x}{t} < \lambda_1(\mathbf{v}_L), \\ \mathbf{v}_L^* & \text{if } \lambda_1(\mathbf{v}_L) < \frac{x}{t} < \lambda_2(\mathbf{v}_L^*), \\ \mathbf{v}_R^* & \text{if } \lambda_2(\mathbf{v}_R^*) < \frac{x}{t} < \lambda_3(\mathbf{v}_R), \\ \mathbf{v}_R & \text{if } \lambda_3(\mathbf{v}_R) < \frac{x}{t}, \end{cases}$$

with

$$\lambda_2(\mathbf{v}_L^*) = \lambda_2(\mathbf{v}_R^*) = u^*.$$

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Setting

$$\begin{split} u_{L}^{*} &= u_{R}^{*} = u^{*}, \\ \tau_{L}^{*} &= \tau_{L} + (u^{*} - u_{L})/a, \\ \tau_{R}^{*} &= \tau_{R} - (u^{*} - u_{R})/a, \\ (\rho_{i})_{L}^{*} &= (\rho_{i})_{L} \tau_{L}/\tau_{L}^{*}, \quad i = 1, ..., n, \\ (\rho_{i})_{R}^{*} &= (\rho_{i})_{R} \tau_{R}/\tau_{R}^{*}, \quad i = 1, ..., n, \\ \Pi^{*} &= \Pi_{L}^{*} &= \Pi_{R}^{*} = \frac{1}{2}(\Pi_{L} + \Pi_{R}) - \frac{a}{2}(u_{R} - u_{L}), \\ (e_{\nu,j})_{L}^{*} &= (e_{\nu,j})_{L}, \quad j = 1, ..., n\nu, \\ (e_{\nu,j})_{R}^{*} &= (e_{\nu,j})_{R}, \quad j = 1, ..., n\nu, \\ (S_{e})_{L}^{*} &= (S_{e})_{L}, \\ (S_{e})_{R}^{*} &= (S_{e})_{R}, \\ E_{L}^{*} &= E_{L} + (\Pi_{L}u_{L} - \Pi^{*}u^{*})/a, \\ E_{R}^{*} &= E_{R} - (\Pi_{R}u_{R} - \Pi^{*}u^{*})/a, \end{split}$$

the intermediate states are defined by :

$$\mathbf{v}_{L}^{*} = \begin{pmatrix} \{(\rho_{i})_{L}^{*}\}_{i=1,...,n} \\ (\rho u)_{L}^{*} \\ (\rho E)_{L}^{*} \\ (\rho S_{e})_{L}^{*} \\ \{(\rho e_{\nu,j})_{L}^{*}\}_{j=1,...,n\nu} \\ (\rho \Pi)_{L}^{*} \end{pmatrix},$$
$$\mathbf{v}_{R}^{*} = \begin{pmatrix} \{(\rho_{i})_{R}^{*}\}_{i=1,...,n} \\ (\rho u)_{R}^{*} \\ (\rho E)_{R}^{*} \\ (\rho S_{e})_{R}^{*} \\ \{(\rho e_{\nu,j})_{R}^{*}\}_{j=1,...,n\nu} \\ (\rho \Pi)_{R}^{*} \end{pmatrix}.$$

Moreover,  $\mathbf{v}_L^*$  and  $\mathbf{v}_R^*$  are in  $\Omega_{\mathbf{v}}$ .

In the notation  $\mathbf{v}_a(x/t; \mathbf{v}_L, \mathbf{v}_R)$ , the subscript  $_a$  highlights the dependence of the solution with respect to the parameter a. In addition, observe that condition (16) gives the characteristic speeds in the Riemann solution with increasing order.

#### Numerical scheme

In this section, we present a relaxation scheme for approximating the weak solutions of the Cauchy problem (12)-(13) with initial data

$$\mathbf{u}(x,0) = \mathbf{u}_0(x).$$

Based on system (15), the procedure is classical within the framework of relaxation method (see for instance, Jin,<sup>16</sup> Coquel and al.<sup>17</sup> or Chalons<sup>13</sup>). It is made of two steps that we describe in details : the first one consists in a time evolution of the solution according to system (15) with  $\lambda = 0$ , while the second one projects the uptaded solution at equilibrium state  $\lambda = +\infty$ . We first set some notations.

Let  $\Delta x$  and  $\Delta t$  be two constant steps for space and time discretizations. Let  $(x_j)_{j\in\mathbb{Z}}$  be a sequence of equidistributed points of  $\mathbb{R}$ :  $x_{j+1} - x_j = \Delta x$ . For all  $j \in \mathbb{Z}$  and all  $n \in \mathbb{N}$ , we introduce the notations

$$x_{j+1/2} = x_j + \frac{\Delta x}{2}, \quad t^n = n\Delta t,$$

and consider the following discretization of the computational domain  $\mathbb{R}_x \times \mathbb{R}_t^+$ :

$$\mathbb{R}_{x} \times \mathbb{R}_{t}^{+} = \bigcup_{j \in \mathbb{Z}} \bigcup_{n \ge 0} C_{j}^{n}, \quad C_{j}^{n} = [x_{j-1/2}, x_{j+1/2}] \times [t^{n}, t^{n+1}]$$

As usual in the context of finite volume methods, the approximate solution  $\mathbf{u}_{\Delta t,\Delta x}(x,t)$  of (12)-(13) with initial data  $\mathbf{u}_0$  is sought as a piecewise constant function on each slab  $C_i^n$ .

$$\mathbf{u}_{\Delta t,\Delta x}(x,t) = \mathbf{u}_j^n \text{ for } (x,t) \in C_j^n,$$

and for the sake of completeness

$$\mathbf{u}_{j}^{0} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{u}_{0}(x) dx, \quad j \in \mathbb{Z}.$$

On the other hand, we also define from  $\mathbf{u}_{\Delta t,\Delta x}$  another piecewise constant approximate solution  $\mathbf{v}_{\Delta t,\Delta x}$ by setting

$$\mathbf{v}_{\Delta t,\Delta x}(x,t) = \mathbf{v}_j^n = \begin{pmatrix} \mathbf{u}_j^n \\ (\rho \Pi)_j^n \end{pmatrix}$$
 for  $(x,t) \in C_j^n$ .

This solution is set to be at equilibrium, that is

$$(\rho\Pi)_j^n = (p+p_e)(\mathbf{u}_j^n).$$

Let us assume as known the solution  $\mathbf{u}_{\Delta t,\Delta x}(x,t^n)$  at time  $t^n$ . In order to advance it to the next time level  $t^{n+1}$ , we now precise each of the two steps of the algorithm.

First step : evolution in time  $(t^n \rightarrow t^{n+1-})$ 

In this step, we take  $\lambda = 0$  and solve system (15) with  $\mathbf{v}_{\Delta t,\Delta x}(x,t^n)$  as initial data and for times  $t \in [0,\Delta t]$ . Under CFL condition

$$\frac{\Delta t}{\Delta x} \max_{\mathbf{v}}(|\lambda_i(\mathbf{v})|, i=1,2,3) < \frac{1}{2}, \tag{18}$$

where the maximum is taken over all the **v** under consideration, the solution is obtained by solving a sequence of non interacting Riemann problems set at each cell interface  $x_{j+1/2}$ , and so is actually known thanks to theorem 1. Note that *a* can be chosen locally in space, i.e. with a value that possibly differs from one interface to another. If  $a_{j+1/2}$  denotes the value of *a* for the Riemann problem set at interface  $x_{j+1/2}$ , we have :

$$\mathbf{v}(x,t) = \mathbf{v}_{a_{j+1/2}}\left(\frac{x-x_{j+1/2}}{t}; \mathbf{v}_j^n, \mathbf{v}_{j+1}^n\right),$$
  
for  $(x,t) \in [x_j, x_{j+1}] \times ]0, \Delta t], \quad j \in \mathbb{Z}$ .

As it is usually done, we propose to get back a piecewise constant function in  $x \in [x_{j-1/2}, x_{j+1/2}]$  by means of a  $L^2$  projection :

$$\begin{split} \tilde{\mathbf{v}}(x,t) &= \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{v}(x,t) dx,\\ \text{for } (x,t) &\in [x_{j-1/2}, x_{j+1/2}] \times ]0, \Delta t], \ j \in \mathbb{Z}. \end{split}$$

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We then complete this first step by setting

$$\mathbf{v}_{j}^{n+1-} = \begin{pmatrix} \mathbf{u}_{j}^{n+1-} \\ (\rho\Pi)_{j}^{n+1-} \end{pmatrix} = \tilde{\mathbf{v}}(x_{j}, \Delta t), \quad j \in \mathbb{Z}.$$
(19)

Of course, this procedure is nothing but the celebrated Godunov method applied to (15). As a consequence, updated formula (19) equivalently recasts according to the following conservation form

$$\mathbf{v}_{j}^{n+1-} = \mathbf{v}_{j}^{n} - \frac{\Delta t}{\Delta x} (g(\mathbf{v}_{j}^{n}, \mathbf{v}_{j+1}^{n}) - g(\mathbf{v}_{j-1}^{n}, \mathbf{v}_{j}^{n})),$$
$$j \in \mathbb{Z}, \quad n \ge 0,$$
(20)

where the numerical flux function writes

$$g(\mathbf{v}_{j}^{n}, \mathbf{v}_{j+1}^{n}) = \mathcal{F}(\mathbf{v}_{a_{j+1/2}}(0; \mathbf{v}_{j}^{n}, \mathbf{v}_{j+1}^{n})).$$
(21)

Let us recall that the numerical flux (21) is here explicitly known.

Before presenting the second step of the algorithm, we briefly discuss the definition of the parameter  $a_{j+1/2}$ in the numerical flux (21). It is known from literature<sup>14, 15</sup> that each value  $a_{j+1/2}$  has to be carefully chosen. In order to avoid instabilities in the relaxation procedure as  $\lambda$  goes to infinity, some compatibility conditions with respect to the original system (12) have to be satisfied. These conditions, often referred as to sub-characteristic conditions or Whitham conditions, express that each characteristic speed of the relaxation model (15) with  $\lambda = 0$  must be greater than the corresponding one in the equilibrium system (12), that is  $a > \rho c$  (see indeed propositions 1 and 2). ¿From a numerical point of view, we propose to impose

$$a_{j+1/2} > \max(\{\rho c\}(\mathbf{u}_{j}^{n}), \{\rho c\}(\mathbf{u}_{j+1}^{n})).$$
 (22)

At each interface, the parameter a can thus a priori be selected unspecified in the infinite domain described by relation (22). However, a deeper analysis of the relaxation system (14) would demonstrate that the associated rate of entropy dissipation actually depends on this parameter. In fact, this rate increases with a. As a consequence, this parameter should be chosen as small as possible according to (22) in order to lower the numerical dissipation. This is the main motivation in the use of a local definition.

## Second step : relaxation $(t^{n+1-} \rightarrow t^{n+1})$

We now project the solution  $\mathbf{v}_{\Delta t,\Delta x}(x, t^{n+1-})$ obtained at the end of the previous step on the equilibrium manifold  $\lambda = +\infty$ . More precisely, we set for all  $j \in \mathbb{Z}$ :

$$\mathbf{v}_{j}^{n+1} = \begin{pmatrix} \mathbf{u}_{j}^{n+1} \\ (\rho\Pi)_{j}^{n+1} \end{pmatrix} \quad \text{with} \quad \mathbf{u}_{j}^{n+1} = \mathbf{u}_{j}^{n+1-1}$$
  
and  $(\rho\Pi)_{j}^{n+1} = (p+p_{e})(\mathbf{u}_{j}^{n+1}).$ 
(23)

Such an operation can be seen as a rough but efficient manner of bringing  $\mathbf{v}_{\Delta t,\Delta x}(x,t^{n+1-})$  closer to the equilibrium system (12). Indeed,  $\mathbf{v}_{\Delta t,\Delta x}(x,t^{n+1-})$  is in general far from an equilibrium state and so cannot be considered as a fair approximation of the solution of (12). In addition, updating formula (23) are equivalent to solve the following ordinary differential equations system with  $\lambda = +\infty$ :

$$\begin{cases} \partial_{t}\rho_{i} = 0, \quad i = 1, ..., n, \\ \partial_{t}(\rho u) = 0, \\ \partial_{t}(\rho E) = 0 \\ \partial_{t}(\rho S_{e}) = 0, \\ \partial_{t}(\rho_{j}e_{v,j}) = 0, \quad j = 1, ..., n\nu, \\ \partial_{t}(\rho \Pi) = \lambda \rho(p + p_{e} - \Pi), \end{cases}$$
(24)

so that the whole algorithm may be understood as a splitting strategy applied on (15) : we solve first the convective part and, afterwards, we consider the source term in the regime  $\lambda \to \infty$ .

In agreement with the description of these two steps, the approximate solution  $\mathbf{u}_{\Delta t,\Delta x}$  is then updated according to the following consistent finite volume method:

$$\begin{split} \mathbf{u}_{j}^{n+1} &= \mathbf{u}_{j}^{n} - \frac{\Delta t}{\Delta x} (f(\mathbf{u}_{j}^{n}, \mathbf{u}_{j+1}^{n}) - f(\mathbf{u}_{j-1}^{n}, \mathbf{u}_{j}^{n})), \\ & j \in \mathbb{Z}, \quad n \geq 0, \end{split}$$

where the numerical flux  $f(\mathbf{u}_{j}^{n}, \mathbf{u}_{j+1}^{n})$  is given by the N first components of the consistent numerical flux function  $g(\mathbf{v}_{j}^{n}, \mathbf{v}_{j+1}^{n})$ .

We conclude this section by emphasizing that several stability properties are met by this relaxation scheme. For instance, a discrete version of entropy inequality (13) can be obtained. Such a result is pretty technical to establish and so is not presented in this paper. We refer the reader to a follow-up paper from the authors, and to Chalons<sup>13</sup> for similar results in a slightly different context. Notice that a refinement of the Whitham condition (22) is needed. In addition, expected discrete maximum principles also hold on  $S_e$  and  $\{e_{v,j}\}_{j=1,...,n\nu}$ .

#### Numerical Experiments

The gas mixture under consideration contains three species, namely nitrogen atoms N, nitrogen ions N<sup>+</sup> and electrons. Three shocktube testcases have been considered and the description of the initial left and right states are given in tables 1,2,3. Note that we only need to prescribe the mass fraction of the nitrogen atoms since the other concentrations comes from the local charge neutrality and the relationship  $\sum_{i=1}^{n} Y_i + Y_e = 1$ . The conditions have been chosen in order to get different types of waves. The results are presented in Fig. 1,2,3. For each testcase, we show

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Table 1	Testcase A	A definition	
	Left state	Right state	
u(m/s)	1500	-2000	
p(Pa)	$7.5 x 10^4$	$1.5 x 10^4$	
T(K)	4000	1378	
$T_e(K)$	6000	1000	
$\mathbf{Y}_N$	0.7999998	0.8999998	
Table 2         Testcase B definition			
	Left	Right	
u(m/s)	2200	0	
p(Pa)	$1x10^{4}$	$5x10^{5}$	
T(K)	780	4742	
$T_e(K)$	2000	8300	
$\mathbf{Y}_N$	0.7999999	0.8989998	
Table 3 Testcase C definition			
	Left	Right	
u(m/s)	0	-1500	
p(Pa)	$3x10^{5}$	$6.5 \times 10^{3}$	
T(K)	2452	346	
$T_e(K)$	8000	300	
$\mathbf{Y}_N$	0.8998999	0.7989998	

the heavy species pressure, the electron pressure and the total pressure  $p + p_e$  and we compare the distributions obtained with a Godunov solver, the previous Roe scheme and the relaxation scheme. Results are in good agreement even if some discrepancies appear in the region of the 2-wave (contact discontinuity) for the heavy species pressure and the electron pressure. Note that, as it is expected from the mathematical properties of the system, the variable  $p + p_e$  is constant through the contact discontinuity.

#### **Concluding Remarks**

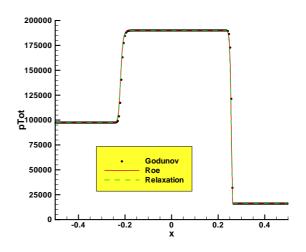
The paper presents a relaxation model developed for the numerical approximation of weakly ionized flows in the context of hypersonic hyperenthalpic flows. Governing equations rest on a conservative system proposed by Coquel and Marmignon. Comparisons between different solvers for shocktube applications assess the relaxation approach since the results comparison with a Godunov solver and a Roe solver is fair. Extension of the relaxation model to two dimensional configurations is now planned.

#### References

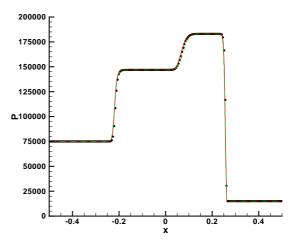
<sup>1</sup>Candler, G. and MacCormack, R., "The Computation of Hypersonic Ionized Flows in Chemical and Thermal Nonequilibrium," AIAA Paper 88–0511, 1988.

<sup>2</sup>Josulya, E. and Bailey, W. F., "Governing Equations for Weakly Ionized Plasmas Flowfields of Aerospace Vehicles," AIAA Paper 2002–2228, 2002.

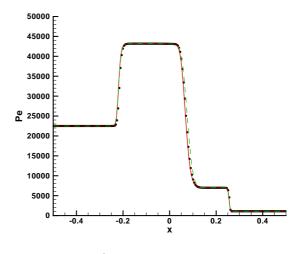
<sup>3</sup>Walpot, L., *Development and Application of a Hypersonic Flow Solver*, Phd thesis, Technische Universiteit Delft, 2002.



a) Total pressure  $(p + p_e)$ .



b) Heavy species pressure.

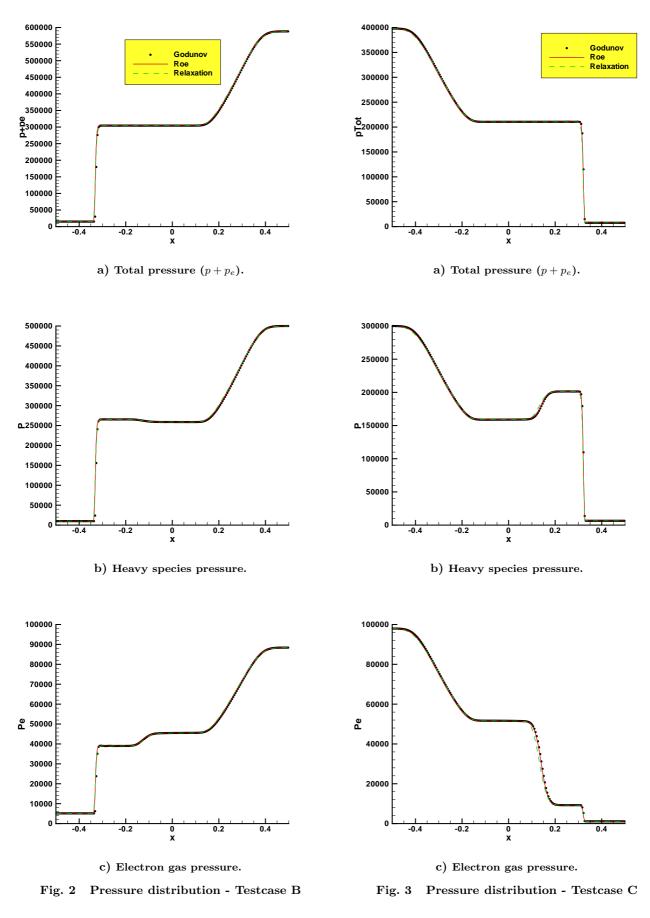


c) Electron gas pressure.



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<sup>4</sup>Tchuen, G., Modélisation et Simulation numérique des écoulements à haute enthalpie: influence du déséquilibre électronique, Phd thesis, Université de Provence Aix-Marseille I, 2003.

<sup>5</sup>Soubrié, T. and Rouzaud, O., "Computation of Weakly Multi-Ionized Gases for Atmospheric Entry using an Extended Roe Scheme," Proceedings, 2004, In ECCOMAS Conference Proceedings.

<sup>6</sup>Appleton, J. and Bray, K., "The Conservation Equations for a Non-Equilibrium Plasma," *J. Fluid Mech.*, Vol. 20, No. 4, 1964, pp. 659–672.

<sup>7</sup>Lee, J. H., "Basic Governing Equations for the Flight Regimes of Aeroassisted Orbital Transfer Vehicles," AIAA Paper 84–1729, 1984.

<sup>8</sup>Hou, T. and LeFloch, P., "Why Non-Conservative Schemes Converge to Wrong Solutions: Error Analysis," *Math. of Comp.*, Vol. 62, No. 206, 1994, pp. 497–530.

<sup>9</sup>Karni, S., "Maximum principle on the entropy and second order kinetic schemes," *SIAM J. Num. Anal.*, Vol. 29, No. 6, 1992, pp. 1592–1609.

<sup>10</sup>P.A., R. and L., S., "A Non-Conservative Hyperbolic System modelling Spray Dynamics. Part 2: Existence of Travelling Wave Solutions," *SIAM J. Appl. Anal.*, Vol. 56, 1995.

<sup>11</sup>Berthon, C., Contribution à l'analyse numérique des équations de Navier-Stokes compressibles à deux entropies spécifiques, Phd thesis, Université Paris VI, 1999.

 $^{12}\mathrm{Coquel},$  F. and Marmignon, C., "A voir," ONERA Report RSF. no 6/1929AY, 1993.

<sup>13</sup>Chalons, C., Bilans d'entropie discrets dans l'approximation numérique des chocs non classiques. Application aux équations de Navier-Stokes multi-pression 2D et à quelques systèmes visco-capillaires, Phd thesis, Ecole polytechnique, 2002.

<sup>14</sup>Liu, T. P., "Hyperbolic conservation laws with relaxation," Comm. Math. Phys., Vol. 108, 1987, pp. 153–175.

<sup>15</sup>Chen, G. Q., Levermore, C. D., and Liu, T. P., "Hyperbolic conservation laws with stiff relaxation terms and entropy," *Comm. Pure Appl. Math*, Vol. 48, No. 7, 2003, pp. 787–830.

<sup>16</sup>Jin, S. and Xin, Z., "The Relaxation Schemes for Systems of Conservation Laws in Arbitrary Space Dimension," *Comm. Pure. Appl. Math.*, Vol. 48, 1995, pp. 235–276.

<sup>17</sup>Coquel, F., Godlewski, E., In, A., Perthame, B., and Rascle, P., "Some new Godunov and relaxation methods for two phase flows," *Proceedings of an International conference* on Godunov methods : Theory and Applications, Kluwer Academic/Plenum Publishers, 2001.