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A MODEL AND A NUMERICAL SCHEME TO COMPUTE LAMINAR FLAMES IN DUST SUSPENSIONS

M. D'AMICO*, O. DUFAUD†, D. GRAPSAS‡, AND J.-C. LATCHÉ*

Abstract. We address in this paper a system of balance equations which models the low Mach number one-dimensional reactive flow generated by the combustion of a dust suspension. This model features rather general diffusion terms, with, in particular, mass diffusion coefficients which depend on the local composition and differ in function of the considered chemical species. For the solution of this system, we develop a fractional step finite volume algorithm which preserves by construction the stability properties of the continuous problem, namely the positivity of the chemical species mass fractions, the fact that they sum is equal to one, and the non-decrease of the temperature, provided that the chemical reaction is exothermic.

Key words. finite volumes, staggered, reactive flows, dust combustion.

1. Introduction. We address in this paper a model for the combustion of dust suspensions. This model is dedicated to the simulation of laminar flames, for which a one-dimensional representation, supposing a low Mach number flow, is sufficient. Particular care has to be paid to the formulation of the diffusion fluxes, since they determine the structure of the flame; in particular, the mass diffusion coefficients depends on the local composition of the mixture, and differ from one chemical species to another one. Consequently, (standard) simplifications performed to derive the model will yield balance equation for the mass of the chemical species which preserve the positivity of the mass fractions and the fact that their sum is equal to 1, but does not satisfy a maximum principle (*i.e.* non-physical local accumulation of a species can not be excluded). On the opposite, the energy balance equation does satisfy a maximum principle so, provided that the chemical reaction is exothermic, the minimal temperature cannot decrease. The aim of this paper is to develop a fractional-step finite volume scheme for the solution of this problem, to show that it has at least one solution and that any possible solution satisfies the above-mentioned physical bounds.

The exposition is structured as follows. The physical model is introduced in the next section, then the scheme is given in Section 3. Its properties are analysed in Section 4.

2. The physical model. We first give the balance equations, then the closure laws for the mass diffusion terms.

2.1. The system of balance equations. The flow is supposed to be governed by the balance equations modelling a variable density flow in the asymptotic limit of low Mach number flows, namely the mass balance of the chemical species and of the mixture, the enthalpy balance, and the momentum balance equations. For a one-dimensional flow in such a quasi-incompressible situation, the role played by the mass and momentum balance equations is quite different than in the multi-dimensional case: indeed, since, in one space dimension, both the divergence and the gradient

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may be considered as transport operators, the velocity may be seen as the solution of the mass balance equation, and the momentum balance yields the dynamic pressure. Since this latter unknown does not appear in the other equations, its computation is of poor interest, and the momentum balance equation may be disregarded.

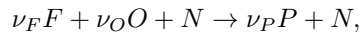
Except for this aspect, equations in this section are written in the usual multi-dimensional form. The computational domain is denoted by Ω , and its boundary $\partial\Omega$ is supposed to be split in an inflow part $\partial\Omega_I$ (where the flow enters the domain, *i.e.* $\mathbf{u} \cdot \mathbf{n}_{\partial\Omega} \leq 0$, with \mathbf{u} the flow velocity and $\mathbf{n}_{\partial\Omega}$ the normal vector to $\partial\Omega$ outward Ω) and an outflow one $\partial\Omega_O$ (where the flow leaves the domain, *i.e.* $\mathbf{u} \cdot \mathbf{n}_{\partial\Omega} \geq 0$) of positive $(d-1)$ -measure, with $\partial\Omega = \partial\Omega_I \cup \partial\Omega_O$ and $\partial\Omega_I \cap \partial\Omega_O = \emptyset$. The problem is supposed to be posed over the time interval $[0, T]$.

Mass balance equations – The mass balance reads:

$$\partial_t(\rho) + \operatorname{div}(\rho\mathbf{u}) = 0, \quad (2.1)$$

where ρ stands for the fluid density. This equation must be complemented by an initial condition ρ_0 , and the density ρ must be given on the inflow part of the boundary, which we denote by $\rho = \rho_I$ on $\partial\Omega_I$. Both functions ρ_0 and ρ_I are supposed to be positive, and the solution of (2.1) may be shown to be positive too.

Only four chemical species are supposed to be present in the flow, namely the dust, or fuel (denoted by F), the oxydant (O), the product (P) of the reaction, and a neutral gas (N). A one-step irreversible total chemical reaction is considered, which is written:



where ν_F , ν_O and ν_P are the molar stoichiometric coefficients of the reaction. The system of the mass balance equations for the chemical species reads:

$$\partial_t(\rho y_i) + \operatorname{div}(\rho y_i \mathbf{u}) + \operatorname{div}(\mathbf{j}_i) = \dot{\omega}_i, \quad \text{for } 1 \leq i \leq N_s, \quad (2.2)$$

where y_i , \mathbf{j}_i and $\dot{\omega}_i$ stand respectively for the mass fraction, the mass diffusion flux and the reaction rate of the species i . The number of species is denoted by N_s , with, by assumption, $N_s = 4$, and we indifferently use the notation $(y_i)_{1 \leq i \leq N_s}$ or y_F , y_O , y_P and y_N for the fuel, oxydant, product and neutral gas mass fractions, respectively. System (2.2) must be complemented by initial and boundary conditions for $(y_i)_{1 \leq i \leq N_s}$. At the inflow boundary, the total flux (*i.e.* the sum of the convection and of the diffusion fluxes) is prescribed and, at the outflow boundary, the diffusion flux is supposed to vanish:

$$\text{on } \partial\Omega_I, \quad (\rho y_i \mathbf{u} + \mathbf{j}_i) \cdot \mathbf{n}_{\partial\Omega} = (y_i)_I \mathbf{u} \cdot \mathbf{n}_{\partial\Omega}, \quad (2.3a)$$

$$\text{on } \partial\Omega_O, \quad \mathbf{j}_i \cdot \mathbf{n}_{\partial\Omega} = 0. \quad (2.3b)$$

The prescribed values of the mass fractions $(y_i)_{1 \leq i \leq N_s}$ at the initial time and the quantities $((y_i)_I)_{1 \leq i \leq N_s}$ given on the inflow boundary lie in the interval $[0, 1]$.

The reaction rate of each chemical species may be written as:

$$\dot{\omega}_F = \nu_F W_F \dot{\omega}, \quad \dot{\omega}_O = \nu_O W_O \dot{\omega}, \quad \dot{\omega}_P = -\nu_P W_P \dot{\omega} \quad \text{and} \quad \dot{\omega}_N = 0,$$

where W_F , W_O and W_P stand for the molar masses of the fuel, oxydant and product respectively, and $\dot{\omega}$ is a non-negative reaction rate, which is supposed to vanish when either $y_F = 0$ or $y_O = 0$. Since $\nu_F W_F + \nu_O W_O = \nu_P W_P$, we have:

$$\dot{\omega}_F + \dot{\omega}_O + \dot{\omega}_P = 0. \quad (2.4)$$

Since the From a computational point of view, it is convenient to resolve an

The sum of the mass diffusion fluxes of the chemical species is supposed to vanish everywhere in Ω :

$$\sum_{i=1}^{N_s} \mathbf{j}_i = 0. \quad (2.5)$$

In addition, for $1 \leq i \leq N_s$, we assume that the operators $y_i \mapsto \operatorname{div}(\mathbf{j}(y_i))$ are "positivity-preserving", so Equation (2.2), with the fact that the reaction rates vanish when the mass fractions vanish and with positivity assumptions on initial and boundary conditions, only has non-negative solutions.

Let the variable Σ stand for $\Sigma = \sum_{i=1}^{N_s} y_i$. Summing the chemical species mass balance equations (2.2) and using relations (2.4) and (2.5) yields:

$$\partial_t(\Sigma\rho) + \operatorname{div}(\Sigma\rho\mathbf{u}) + \operatorname{div}\left(\sum_{i=1}^{N_s} \mathbf{j}_i\right) = \dot{\omega}_F + \dot{\omega}_O + \dot{\omega}_P,$$

and thus, by (2.4) and (2.5),

$$\partial_t(\Sigma\rho) + \operatorname{div}(\Sigma\rho\mathbf{u}) = 0. \quad (2.6)$$

We now suppose that the quantity Σ is prescribed to 1 at the initial time and at the boundaries (*i.e.* that $\sum_{i=1}^{N_s} (y_i)_0(\mathbf{x}) = 1$ a.e. in Ω and that $\sum_{i=1}^{N_s} (y_i)_I(\mathbf{x}, t) = 1$ a.e. in $\partial\Omega_I \times (0, T)$). Then, using the mass balance equation (2.1) to recast (2.6) under its so-called non-conservative form, we obtain that $\Sigma = 1$ is solution. Provided that the problem (2.6) is regular (*i.e.* admits only one solution), relation (2.6) thus implies that $\Sigma(\mathbf{x}, t) = 1$ for any $\mathbf{x} \in \Omega$ and $t \in [0, T]$. Note that, together with the fact that $y_i \geq 0$, for $1 \leq i \leq N_s$, this implies that $y_i \leq 1$.

Energy balance – In the low Mach number approximation (*i.e.* neglecting the work of the pressure forces because of the quasi-incompressibility of the flow) and disregarding the viscous dissipation, the total enthalpy balance reads:

$$\sum_{i=1}^{N_s} c_{p,i} \left[\partial_t(\rho y_i \theta) + \operatorname{div}(\rho y_i \theta \mathbf{u}) + \operatorname{div}(\theta \mathbf{j}_i) \right] - \operatorname{div}(\lambda \nabla \theta) = \dot{\omega}_\theta, \quad (2.7)$$

where θ stands for the temperature, $c_{p,i}$ for the specific heat of the species i (supposed to be constant) and $\dot{\omega}_\theta$ is the heat production rate due to the chemical reaction. This latter term reads:

$$\dot{\omega}_\theta = - \sum_{i=1}^{N_s} \Delta h_{f,i}^0 \dot{\omega}_i, \quad (2.8)$$

with $\Delta h_{f,i}^0$ denoting the formation enthalpy of the chemical species i at 0°K . This equation must be complemented by a positive initial condition for the temperature and boundary conditions. Once again, we assume a total flux condition at the inlet boundary, and that the diffusion flux vanishes at the outlet boundary:

$$\text{on } \partial\Omega_I, \quad \sum_{i=1}^{N_s} c_{p,i} \theta (\rho y_i \mathbf{u} + \mathbf{j}_i) \cdot \mathbf{n}_{\partial\Omega} = \sum_{i=1}^{N_s} c_{p,i} \rho (y_i)_I \theta_I \mathbf{u} \cdot \mathbf{n}_{\partial\Omega}, \quad (2.9a)$$

$$\text{on } \partial\Omega_O, \quad -\lambda \nabla \theta \cdot \mathbf{n}_{\partial\Omega} = 0 \quad (\text{and } \mathbf{j}_i \cdot \mathbf{n}_{\partial\Omega} = 0 \text{ by (2.3b)}), \quad (2.9b)$$

where θ_I stands for a positive function defined on $\partial\Omega_I \times (0, T)$. Once again, thanks to the species mass balance equations (2.2), we can obtain the so-called non-conservative form of the enthalpy balance (2.7), which reads:

$$\left[\sum_{i=1}^{N_s} c_{p,i} y_i \right] \rho \partial_t \theta + \left[\sum_{i=1}^{N_s} c_{p,i} (\rho y_i \mathbf{u} + \mathbf{j}_i) \right] \cdot \nabla \theta - \text{div}(\lambda \nabla \theta) = \dot{\omega}_\theta. \quad (2.10)$$

Let $\underline{\theta} > 0$ be defined as the minimum value of θ_0 on Ω and of θ_I on $\partial\Omega_I \times (0, T)$. The left-hand side of the preceding relation may be seen as a transport-diffusion operator applied to θ ; since this operator satisfies a maximum principle, supposing that the chemical reaction is exothermic (*i.e.* $\dot{\omega}_\theta \geq 0$), we obtain that $\theta(\mathbf{x}, t) \geq \underline{\theta}$ for a.e. $(\mathbf{x}, t) \in \Omega \times (0, T)$.

Equation of state – Finally, we must give an equation of state to close the system. Let us denote by ρ_i the density of the component i , let \mathcal{I}_s be the set of indices corresponding to solid species and \mathcal{I}_g the set of the indices corresponding to gaseous species (so $\mathcal{I}_s \cup \mathcal{I}_g = \{1, \dots, N_s\}$). We suppose that the gas phase is a mixture of perfect gases. Assuming that the density of the solid phase is constant, the usual mixture law reads:

$$\rho = \varrho(\theta, (y_i)_{1 \leq i \leq N_s}) = \frac{1}{\frac{R\theta}{P_{th}} \sum_{i \in \mathcal{I}_g} \frac{y_i}{W_i} + \sum_{i \in \mathcal{I}_s} \frac{y_i}{\rho_i}}, \quad (2.11)$$

where $R = 8.31451 \text{ JK}^{-1} \text{ mol}^{-1}$ stands for the perfect gases constant. Since we assumed that the measure of $\partial\Omega_O$ is positive (*i.e.* the computational domain is not closed), the so-called thermodynamic pressure P_{th} is constant in time and space, and given by the initial state.

2.2. Expression of the chemical species diffusion fluxes. Since the size of the particles is large compared to the molecular Brownian motion ranges, we suppose that the diffusion of dusts vanishes, so the diffusion phenomena only occur in the gas phase. We define the gas mass fraction as $y_g = \sum_{i \in \mathcal{I}_g} y_i$ and, for $i \in \mathcal{I}_g$, the mass fraction of the species i in the gas phase as $\tilde{y}_i = y_i / y_g$. A general expression of the diffusion fluxes read:

$$\text{for } i \in \mathcal{I}_s, \quad \mathbf{j}_i = 0; \quad \text{for } i \in \mathcal{I}_g, \quad \mathbf{j}_i = -\rho \sum_{j \in \mathcal{I}_g} D_{i,j} \nabla \tilde{y}_j,$$

where the coefficients $(D_{i,j})_{i,j \in \mathcal{I}_g}$ depend on the local mixture concentration (*i.e.* on the mass fractions $(\tilde{y}_i)_{i \in \mathcal{I}_g}$ themselves). However, using a full tensor D and computing its coefficients is cost-consuming, and, moreover, the complete data necessary

to their accurate computation is usually not available. This tensor is thus generally approximated. For instance, a "quasi-diagonal" approximation to this purpose for pure gaseous mixtures reads:

$$\text{for } i \in \mathcal{I}_g, \quad \mathbf{j}_i = \mathbf{j}_i^e + \tilde{y}_i \mathbf{J}, \quad \mathbf{j}_i^e = -\rho D_i \frac{W_i}{W} \nabla \tilde{x}_i,$$

where \tilde{x}_i stands for the molar mass fraction of the component i , so

$$\tilde{x}_i = \tilde{y}_i \frac{W}{W_i}, \quad \text{with } \frac{1}{W} = \sum_{i \in \mathcal{I}_g} \frac{\tilde{y}_i}{W_i}. \quad (2.12)$$

The quantity W is the so-called gaseous mixture molar mass. Complemented by a suitable expression of the coefficient D_i (see Equation (2.13) below), this formula is known as the Hirschfelder and Curtiss approximation (see [1, 2] and [4, pp. 14-15]). The term $\tilde{y}_i \mathbf{J}$ is a correction term added to ensure that $\sum_{j=1}^{N_s} \mathbf{j}_j = \sum_{j \in \mathcal{I}_g} \mathbf{j}_j = 0$, and so a suitable expression for \mathbf{J} reads $\mathbf{J} = -\sum_{j \in \mathcal{I}_g} \mathbf{j}_j^e$ (note that, by definition, $\sum_{i \in \mathcal{I}_g} \tilde{y}_i = 1$). Under the Hirschfelder and Curtiss approximation, the diffusion coefficients read:

$$\text{for } i \in \mathcal{I}_g, \quad D_i = \frac{1 - \tilde{y}_i}{\sum_{j \in \mathcal{I}_g, j \neq i} \frac{\tilde{x}_j}{D_{ji}}}, \quad (2.13)$$

where D_{ji} is the binary diffusion coefficient of the species j into species i . Exploiting the expression (2.12) of the molar fractions as a function of the mass fractions, we obtain the following expression for the diffusion fluxes:

$$\text{for } i \in \mathcal{I}_g, \quad \mathbf{j}_i^e = -\rho D_i \frac{1}{y_g} \nabla y_i - \rho D_i y_i \left[\nabla \left(\frac{1}{y_g} \right) + \frac{1}{y_g} \nabla (\log(W)) \right]. \quad (2.14)$$

In this model, the operator $y_i \mapsto \mathcal{D}(y_i) = \text{div}(\mathbf{j}(y_i))$ thus splits in two parts:

$$\mathcal{D}(y_i) = \mathcal{D}_1(y_i) + \mathcal{D}_2(y_i), \quad \mathcal{D}_1(y_i) = -\text{div}(\rho D_i \frac{1}{y_g} \nabla y_i), \quad \mathcal{D}_2(y_i) = -\text{div}(y_i \mathbf{q}_d),$$

with:

$$\mathbf{q}_d = \rho D_i \left[\nabla \left(\frac{1}{y_g} \right) + \frac{1}{y_g} \nabla (\log(W)) \right] - \frac{1}{y_g} \mathbf{J}.$$

The operator \mathcal{D}_1 satisfies a maximum principle, while \mathcal{D}_2 is only positivity-preserving, since the divergence of the vector \mathbf{q}_d is not zero in the general case. For instance, this means that, because of the approximation made for the diffusion tensor, the dust mass fraction may locally exceed the maximum of its initial and boundary values, which is of course unphysical (within the frame of the present model, where a possible drift of the particles with respect to the bulk flow velocity is not taken into account). Hopefully, the occurrence of this phenomenon may be limited in time and space.

3. The numerical scheme. Let us consider a partition $0 = t_0 < t_1 < \dots < t_N = T$ of the time interval $(0, T)$, which we suppose uniform. Let $\delta t = t_{n+1} - t_n$ for $n = 0, 1, \dots, N-1$ be the constant time step. We suppose that the interval Ω is split in a family of control volumes (sub-intervals of Ω) which realizes a partition

of Ω ; we denote these control volumes by $(K)_{K \in \mathcal{M}}$. The scalar unknowns, *i.e.* the density, mass fractions and temperature, are associated to the control volumes, and the corresponding unknowns read $\rho_K^n, (y_i)_K^n, \theta_K^n$ for $K \in \mathcal{M}$ and $0 \leq n \leq N$. The velocity is discretized at faces of the mesh, which we denote by $(\sigma)_{\sigma \in \mathcal{E}}$, so the corresponding unknowns are u_σ^n for $\sigma \in \mathcal{E}$ and $0 \leq n \leq N$. The set of the internal faces, the external faces (*i.e.* the two faces located on the boundary of Ω) and the faces of K is denoted by $\mathcal{E}_{\text{int}}, \mathcal{E}_{\text{ext}}$ and $\mathcal{E}(K)$ respectively, and the face separating two neighbour cells K and L is denoted by $K|L$. For $K \in \mathcal{M}$, x_K stands for the mass center of K and, for $\sigma = K|L \in \mathcal{E}_{\text{int}}$, we define d_σ by $d_\sigma = |x_K - x_L|$. For short, we use indifferently ρ^n (resp. $(y_i)^n, \theta^n, u^n$) and $(\rho_K^n)_{K \in \mathcal{M}}$ (resp. $((y_i)_K^n)_{K \in \mathcal{M}}, (\theta_K^n)_{K \in \mathcal{M}}, (u_\sigma^n)_{\sigma \in \mathcal{E}}$).

We implement a fractional-step algorithm, which consists in four steps, and reads, supposing that $\rho^{n-1}, \rho^n, (y_i)_{1 \leq i \leq N_s}^n, \theta^n$ and u^n are known:

Chemistry step – Solve for $(y_i)_{1 \leq i \leq N_s}^{n+1}$:

For $1 \leq i \leq N_s, \forall K \in \mathcal{M}$,

$$\frac{1}{\delta t} [\rho_K^n (y_i)_K^{n+1} - \rho_K^{n-1} (y_i)_K^n] + \text{div} [\rho^n y_i^{n+1} \mathbf{u}^n]_K + \text{div} [\mathbf{j}_i^n]_K = (\dot{\omega}_i)_K^{n+1}. \quad (3.1a)$$

Energy balance – Solve for θ^{n+1} :

$\forall K \in \mathcal{M}$,

$$\sum_{i=1}^{N_s} c_{p,i} \left[\frac{1}{\delta t} [\rho_K^n (y_i)_K^{n+1} \theta_K^{n+1} - \rho_K^{n-1} (y_i)_K^n \theta_K^n] + \text{div} [\rho^n y_i^{n+1} \theta^{n+1} \mathbf{u}^n]_K \right. \\ \left. + \text{div} [\theta^{n+1} \mathbf{j}_i^n]_K \right] - \text{div} (\lambda \nabla \theta^{n+1})_K = (\dot{\omega}_\theta)_K^{n+1}. \quad (3.1b)$$

Equation of state – $\rho_K^{n+1} = \rho(\theta_K^{n+1}, ((y_i)_K^{n+1})_{1 \leq i \leq N_s})$, for $K \in \mathcal{M}$. (3.1c)

Mass balance – Solve for \mathbf{u}^{n+1} :

$$\forall K \in \mathcal{M}, \quad \frac{1}{\delta t} [\rho_K^{n+1} - \rho_K^n] + \text{div} [\rho^{n+1} \mathbf{u}^{n+1}]_K = 0. \quad (3.1d)$$

We now give the expression of the fluxes appearing in these relations.

Convection fluxes – The guideline for the definition of the convection fluxes is that we want the numerical scheme to respect "by construction" the physical bounds satisfied by the variables in the continuous case. To this purpose, we first remark that an operator which satisfies a maximum principle must vanish when applied to constant functions. Indeed, denoting by \mathcal{L} such an operator, an initially constant solution ξ to the equation $\partial_t \xi + \mathcal{L}(\xi) = 0$ must remain constant, since the upper and lower bounds of the solution have to be preserved (provided, of course, that boundary conditions are consistent with this constant solution); this yields $\partial_t \xi = 0$ and so $\mathcal{L}(\xi) = 0$. In fact, when \mathcal{L} is a discrete convection operator, using an upwind approximation of the unknown at the faces, this condition of preservation is not only mandatory but also sufficient [3]. In the system under consideration, two such convection operators have to be approximated, namely the convection operator for the species mass balance equations and for the energy balance, and the fact that these operators vanish when applied to constant functions is closely related to the fact that these equations may be recast under the so-called non-conservative form thanks to the mixture mass balance

and to the species mass balance, respectively. So, let the convection fluxes in this latter relation read:

$$\operatorname{div}[\rho \mathbf{u}]_K = \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}(K)} F_{K,\sigma}.$$

We then define the convection fluxes in the species mass balance equations as:

$$\operatorname{div}[\rho y_i \mathbf{u}]_K = \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}(K)} F_{K,\sigma} (y_i)_\sigma^{\text{up}},$$

where $(y_i)_\sigma^{\text{up}}$ stands for the upwind approximation of y_i on the face σ with respect to $F_{K,\sigma}$. Similarly, let the convection and diffusion fluxes in this equation be written as:

$$\operatorname{div}[\rho y_i \mathbf{u}]_K + \operatorname{div}[\mathbf{j}_i]_K = \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}(K)} G_{K,\sigma},$$

where, for short, we skip the index i for the flux $G_{K,\sigma}$. Then, in the energy mass balance,

$$\operatorname{div}[\rho y_i \theta \mathbf{u}]_K + \operatorname{div}[\theta \mathbf{j}_i]_K = \sum_{\sigma \in \mathcal{E}(K)} G_{K,\sigma} \theta_\sigma^{\text{up}},$$

where $\theta_\sigma^{\text{up}}$ stands for the upwind approximation of θ on the face σ with respect to $G_{K,\sigma}$. This upwind discretization for y_i and θ for an internal face $\sigma = K|L$ is defined as follows:

$$\begin{aligned} (y_i)_\sigma^{\text{up}} &= (y_i)_K \text{ if } F_{K,\sigma} \geq 0, & (y_i)_\sigma^{\text{up}} &= (y_i)_L \text{ otherwise,} \\ \theta_\sigma^{\text{up}} &= \theta_K \text{ if } G_{K,\sigma} \geq 0, & \theta_\sigma^{\text{up}} &= \theta_L \text{ otherwise.} \end{aligned}$$

For an external face adjacent to K , lying on the outlet part of the boundary, we have $(y_i)_\sigma^{\text{up}} = (y_i)_K$, which is consistent with the above definition since $F_{K,\sigma}$ is supposed to be non-negative, and $\theta_\sigma^{\text{up}} = \theta_K$, which, once again, is consistent with the upwind definition on the internal faces since the mass species diffusion flux is supposed to vanish, and so $G_{K,\sigma} = F_{K,\sigma} (y_i)_\sigma^{\text{up}}$ has the same sign as $F_{K,\sigma}$, *i.e.* it is also non-negative (provided that we are able to prove that the chemical species mass fractions remain non negative, which is indeed done in Section 4 below). For an external face adjacent to K lying on the inlet part of the boundary, both $(y_i)_\sigma$ and θ_σ are computed as an approximation of the mass fractions and the temperature prescribed on the boundary, and, by similar arguments, both $F_{K,\sigma}$ and $G_{K,\sigma}$ are non-positive.

The mass flux through the face σ reads:

$$F_{K,\sigma} = \rho_\sigma u_{K,\sigma}$$

where $u_{K,\sigma}$ stands for the value of the velocity oriented outward K , *i.e.* $u_{K,\sigma} = u_\sigma$ if K is situated "on the left part" of σ and $u_{K,\sigma} = -u_\sigma$ otherwise, and ρ_σ stands for any reasonable approximation of ρ on σ ; here, we choose a centered approximation: $\rho_\sigma = \frac{1}{2}(\rho_K + \rho_L)$ for $\sigma = K|L$, $\rho_\sigma = \rho_K$ for an outlet external face adjacent to K and ρ_σ is computed from the equation of state as a function of the data for the species mass fractions and the temperature for an inlet external face.

Diffusion fluxes – The mass diffusion fluxes vanish for the solid species. For the gaseous chemical species, we have:

$$\operatorname{div}[\mathbf{j}_i^n]_K = \frac{1}{|K|} \sum_{\sigma=K|L} (J_i^n)_{K,\sigma}.$$

Note that the sum is restricted to the internal faces of K since, by assumption, the diffusion fluxes vanish at the boundaries (more precisely speaking, they are supposed to vanish at the outlet boundary and the total flux is written as a convection flux at the inlet boundary, so already taken into account in the definition of $G_{K,\sigma}$ above). For a scalar variable ξ and an internal face $\sigma = K|L$, let us define $-(\partial_x f(\xi))_{K,\sigma}$ and $\{f(\xi)\}_\sigma$ as:

$$-(\partial_x f(\xi))_{K,\sigma} = \frac{1}{d_\sigma} (f(\xi_K) - f(\xi_L)) \quad \text{and} \quad \{f(\xi)\}_\sigma = \frac{1}{2} (f(\xi_K) + f(\xi_L)).$$

For $i \in \mathcal{I}_g$, we then define $(J_i^d)_{K,\sigma}$ as:

$$(J_i^d)_{K,\sigma} = -\left\{ \rho D_i \frac{1}{y_g} \right\}_\sigma (\partial_x y_i)_{K,\sigma}. \quad (3.2)$$

Note that, in this definition, the quantity $\{\rho D_i / y_g\}_\sigma$ may be replaced by any reasonable approximation of $\rho D_i / y_g$ on the face (so, for instance, by the harmonic mean of the cell approximations of this expression, which may possibly give more accurate results when it varies quickly from cell to cell). Let us then introduce the following quantities:

$$(q_i)_{K,\sigma} = -\left\{ \rho D_i \right\}_\sigma \left(\partial_x \left(\frac{1}{y_g} \right) \right)_{K,\sigma} - \left\{ \rho D_i \frac{1}{y_g} \right\}_\sigma (\partial_x (\log(W)))_{K,\sigma},$$

$$(J_i^c)_{K,\sigma} = (q_i)_{K,\sigma} (y_i)_\sigma^{\text{up}/q_i},$$

where $(y_i)_\sigma^{\text{up}/q_i}$ stands for the upwind approximation of y_i at the face σ with respect to $(q_i)_{K,\sigma}$. Finally, let us denote by $q_{K,\sigma}$ the following quantity:

$$q_{K,\sigma} = \sum_{i \in \mathcal{I}_g} (J_i^d)_{K,\sigma} + (J_i^c)_{K,\sigma}.$$

With this notation, the diffusion flux $(J_i)_{K,\sigma}$ reads:

$$(J_i)_{K,\sigma} = (J_i^d)_{K,\sigma} + (J_i^c)_{K,\sigma} + \frac{(y_i)_\sigma^{\text{up}/q}}{(y_g)_\sigma^{\text{up}/q}} q_{K,\sigma},$$

where $(y_i)_\sigma^{\text{up}/q}$ and $(y_g)_\sigma^{\text{up}/q}$ stand for an upwind approximation at the face σ with respect to $q_{K,\sigma}$ of y_i and y_g respectively. Note that this latter upwinding is performed with respect to the same quantity for all the species, and thus $\sum_{i \in \mathcal{I}_g} (y_i)_\sigma^{\text{up}/q} = (y_g)_\sigma^{\text{up}/q}$.

The discrete heat diffusion term in the enthalpy energy balance reads:

$$-\operatorname{div}[\lambda \nabla \theta^{n+1}]_K = \sum_{\sigma=K|L} H_{K,\sigma}, \quad \text{with} \quad H_{K,\sigma} = \lambda_\sigma (\partial_x \theta)_{K,\sigma},$$

where λ_σ stands for an approximation of the diffusion coefficient λ on σ ; for instance, if λ depend on the temperature, a possible choice is $\lambda_\sigma = \{\lambda(\theta)\}_\sigma$.

4. Properties of the scheme. In this section we prove that, at the discrete level, the mass fractions, the temperature and the density preserve the same physical bounds as at the continuous level. To formulate these results, for any discrete family $(x_K^n)_{K \in \mathcal{M}}^{0 \leq n \leq N}$, we introduce the following notations:

$$\bar{x} = \max_{K \in \mathcal{M}} x_K^0 \quad \underline{x} = \min_{K \in \mathcal{M}} x_K^0,$$

In addition, for $a \in \mathbb{R}$, we denote by a^+ the positive part of a (i.e. $a^+ = \max(a, 0)$).

PROPOSITION 4.1 (Stability). *Let the so-called CFL-number be defined by:*

$$\text{CFL}^n = \max_{1 \leq i \leq N_s} \max_{K \in \mathcal{M}} \frac{\delta t}{|K| \rho_K^{n-1}(y_i)_K} \sum_{\sigma=K|L} \left\{ \rho D_i \frac{1}{y_g} \right\}_\sigma \frac{1}{d_\sigma} + (q_i)_{K,\sigma}^+ + \frac{1}{(y_g)_\sigma^{\text{up}/q}} q_{K,\sigma}^+,$$

where, for short, the time-dependent quantities without time exponent are taken at t_n . Then, under the condition $\text{CFL}^n \leq 1$ for any $0 \leq n < N$, there exists a solution to (3.1) satisfying the following stability results:

- (i) for $1 \leq i \leq N_s$, $(y_i)^{n+1} \in [0, 1]$ and $\sum_{i=1}^{N_s} (y_i)^{n+1} = 1$;
- (ii) $\theta^{n+1} \geq \underline{\theta}$;
- (iii) $\underline{\rho}^{n+1} > 0$ and $\bar{\rho}^{n+1} \leq \max \left\{ \frac{P_{th}}{R\underline{\theta}} W_i, \text{ for } i \in \mathcal{I}_g ; \rho_i, \text{ for } i \in \mathcal{I}_s \right\}$.

Proof. We only give here a sketch of the proof and, to this purpose, we proceed by induction, supposing that the bounds (i)–(iii) hold at t_n .

Assertion (i) – The mass fraction systems of equations read:

$$\forall i \in \mathcal{I}, \forall K \in \mathcal{M}, \quad \mathcal{A}_K^{n+1}(y_i)^{n+1} = \frac{|K|}{\delta t} \rho_K^{n-1}(y_i)_K^n - (\mathcal{D}_i)_{K}^{n+1}(y_i)^n + (\dot{\omega}_i)_{K}^{n+1}, \quad (4.1)$$

where \mathcal{A}_K (respectively $(\mathcal{D}_i)_K$) denotes the K -th line of the discretized convection (respectively diffusion) operator, and $(\mathcal{A})_K^{n+1}(y_i)^{n+1}$ (respectively $(\mathcal{D}_i)_{K}^{n+1}(y_i)^n$) has to be seen as the inner product between this line and the vector $(y_i)^{n+1}$ (respectively $(y_i)^n$). Instead of this system, we consider the following slightly modified problem:

$$\forall i \in \mathcal{I}, \forall K \in \mathcal{M}, \quad \mathcal{A}_K^{n+1}(y_i)^{n+1} = \frac{|K|}{\delta t} \rho_K^{n-1}(y_i)_K^n - (\mathcal{D}_i)_{K}^{n+1}(y_i)^n + \alpha(\dot{\omega}_i^+)_{K}^{n+1},$$

where $\dot{\omega}_i^+ = \dot{\omega}_i((y_j^{n+1})_{j \in \mathcal{I}}^+)$ and $\alpha \in [0, 1]$. Note that, for $\alpha = 1$ and if the chemical species mass fractions are non-negative, we recover (4.1). The matrix \mathcal{A} is a discrete “maximum-preserving” operator in the following sense: firstly, its diagonal entries are positive, the off-diagonal terms are non-positive and thanks to the mass balance equation, the sum of the entries over a line is positive. Thus, \mathcal{A} is invertible and \mathcal{A}^{-1} contains only non-negative entries. Under the CFL condition stated above, the sum of the first two terms at the right hand side yields a linear combination of the $((y_i)_K^n)_{K \in \mathcal{M}}$ with non-negative coefficients; since we suppose that $(y_i)^n \geq 0$, this sum is thus non-negative. If $(\dot{\omega}_i)_{K}^{n+1}$ is non-negative, i.e. for $i = P$ and $i = N$, we thus obtain that $(y_i)^{n+1} \geq 0$. The case $(\dot{\omega}_i)_{K}^{n+1} \leq 0$ is more intricate. We now rewrite this term as:

$$(\dot{\omega}_i^+)_{K}^{n+1} = \frac{(\dot{\omega}_i^+)_{K}^{n+1}}{((y_i)_K^{n+1})^+} ((y_i)_K^{n+1})^+.$$

Passing this term to the left-hand side, we obtain a nonlinear function which may be recast as $\mathcal{A}_K^{n+1}((y_i)^{n+1})(y_i)^{n+1}$, with a matrix \mathcal{A} which is still a “maximum-preserving” matrix, whatever the value of y_i^{n+1} may be. So, once again, we conclude that $(y_i)^{n+1}$ is non-negative.

To show that the sum of the mass fractions is equal to 1, let us add the mass fraction equations. This yields the discretized mass balance system, where each term is multiplied by a factor of $\sum_{i \in \mathcal{I}} y_i$ (at the right time-level), since the reaction rates and the diffusion fluxes cancel by construction:

$$\forall K \in \mathcal{M}, \quad \mathcal{A}_K^{n+1} \left(\sum_{i \in \mathcal{I}} (y_i)^{n+1} \right) = \frac{|K|}{\delta t} \rho_K^{n-1} \sum_{i \in \mathcal{I}} (y_i)_K^n.$$

The operator \mathcal{A} is left unchanged compared to the one treated on the mass fraction equations for $i = P$ and $i = N$, thus regular, and thanks to the mass balance, $\forall K \in \mathcal{M}, \sum_{i \in \mathcal{I}} (y_i)_K^{n+1} = 1$ solves the system. Note that this result implies that all mass fractions are bounded above by 1, since that they are non-negative.

Since these bounds hold for any $\alpha \in [0, 1]$, we conclude to the existence of a non-negative solution, thanks to a topological degree argument. Note that we need here that the functions $(y_j)_{j \in \mathcal{I}}^{n+1} \mapsto \dot{\omega}_i^+$, for $i \in \mathcal{I}$, be continuous over an interval strictly larger than the range of variation of the $(y_j)_{j \in \mathcal{I}}^{n+1}$, *i.e.* strictly greater than $[0, 1]$, and thus that the reaction term vanishes as soon as a mass fraction vanishes, which is verified by assumption.

Assertion (ii) – Once more, the proof consists in remarking that the operator acting to the unknown is maximum-preserving. Indeed, by construction, the contributions of the heat diffusion operator over a line cancel, and thanks to the chemical mass fraction equations, the diagonal is dominant. The right-hand side is positive by definition of the $(\dot{\omega}_i)^{n+1}$, thus the temperature at t_{n+1} admits the same lower bound as at t_n .

Assertion (iii) – By the discrete equation of state, ρ^{n+1} is non-negative since $(y_i)_{i \in \mathcal{I}}^{n+1}$ and θ^{n+1} are non-negative too. The upper bound for ρ^{n+1} is obtained from the same relation with a simple computation. \square

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