University PARIS 13 - Sup-Galilée

Internship report

Staggered-grid numerical algorithm for four equations drift-flux model in a porous media

Sami KOURAICHI

CEA - Commissariat à l'énergie atomique et aux énergies renouvelables
Supervising : Mr. **Anouar MEKKAS**

Acknowledgment

First of all I would like to thank Mr. Anouar MEKKAS for supervising me in my internship, for his availability and all the things I acquired next to him. His assistance and advises were determining factors in this project.

Thanks also to Ms. Edwige RICHEBOIS for hosting me in the Laboratoire de Modélisation et simulation à l'Échelle Composant (LMEC) as well as the lab's members who were extremely kind and friendly.

I wish to extend my thanks and gratitude to Mr. Olivier LAFITTE, Mr. Emmanuel AUDUSSE, Mr.Hakim BOUMAZA and all our teachers for their efforts to make the MACS as amazing as it was. I hope that the results of my work will meet their expectations.

Lastly I would like to express the pleasure I had working and cooperating with my colleague Ms. Tassadit ABDELKADER as well as her supervisor Mr.Michael NDJINGA.

Contents

List of Figures

Nomenclature

Phase variables

Symbol	Signification	Unity
ρ_k	density	$kg.m^{-3}$
α_k	void fraction	1
$\vec{V_k}$	velocity vector	$m.s^{-1}$
e_k	internal energy	$J.kg^{-1}$
$E_k = e_k + \|u_k\|^2/2$	total energy	$J.kg^{-1}$
$h_k = e_k + P/\rho_k$	specific enthalpy	$J.kg^{-1}$
$H_k = h_k + \|u_k\|^2/2$	specific total enthalpy	$J.kg^{-1}$
$\bar{\bar{\sigma}}_k$	viscosity tensor	$kg.m^{-1}.s^{-2}$
$h_{k,sat}$	specific enthalpy at saturation	$J.kg^{-1}$
τ_k	friction force vector	

Mixture variables

Symbol	Signification	Unity
$\rho = \sum \alpha_k \rho_k$	density	$kg.m^{-3}$
$\vec{V} = \frac{\sum \alpha_k \rho_k \vec{V_k}}{\rho}$	velocity vector	$m.s^{-1}$
$\vec{V_r} = \vec{V_v} - \vec{V_l}$	relative velocity	$m.s^{-1}$
$C = \frac{\alpha_v \rho_v}{\rho}$	vapor mass concentration	1
$e = \frac{\sum \alpha_k \rho_k e_k}{\rho}$	internal energy	$J.kg^{-1}$
$E = CE_v + (1-C)E_l$	total energy	$J.kg^{-1}$
$h = \frac{\sum \alpha_k \rho_k h_k}{\rho}$	specific enthalpy	$J.kg^{-1}$
P	pressure	Pa

Other variables

Symbol	Signification	Unity
$\vec{g}$	gravity vector	$m.s^{-2}$
ϕ	porosity	1
F_i	interface friction	1
D_h	hydraulic diameter	m
D_{ch}	heating diameter	m
$\mathbb{L} = h_{v,sat} - h_{l,sat}$	latent heat of vaporization	$J.kg^{-1}$
χ	vaporization flow	1
Φ	thermal flow at the wall	$kg.m^{-2}.s^{-2}$
h_{deb}	enthalpie débitante ???????	$J.kg^{-1}$

Introduction

A 4 equation model is used by the Laboratoire de Modélisation et simulation à l'Échelle Composant (LMEC) in the computing code FLICA4 [1]. It is formulated in a three-dimensional and homogenized context in order to avoid having to distinguish between the fluid and the solid structures that constitute the component of interest(reactor core, steam generator, ...).
This model is solved using the numerical method of Roe on a co-located mesh [3]. This "hyperbolic" method works very well for the high-Mach-number flows ($M > 0.1$). However, its analysis in the case of a low-Mach-number flow ($M << 1$), proves that unless we introduce some modifications the solution doesn't converge when the Mach-number tends to zero. For this reason we apply a "pressure correction".
Although the use of this "pressure correction" is necessary to reach the required precision, it produces some oscillations in space. These spatial oscillations are sometimes critical and may lead to unstable resolutions or even divergence in some cases. The purpose of this project is to study another numerical method to avoid the problems we have with the Roe scheme.
This internship was held in the CEA in saclay (Commissariat à l'Énergie Atomique et aux énergies renouvelables) precisely in the LMEC.
In a first step an "elliptic" numerical method is studied. It is used in the computing code CATHARE [2] to solve a two-phase 6 equation model. Then we adapt this method as an alternative to the Roe scheme in order to solve the 4 equation model.

In the first chapter of this report we explain how do we establish the 4 equation model starting from the 6 equation model. In the second chapter we detail the spatial and temporal discretization of the 4 equations. In the third chapter we describe and compare the two solving methods that we tested. In the last chapter are presented the different numerical tests in 1D.

Chapter I

Establishment of the porous 4 equations model

I.1 Porous 6 equations model

The local Navier-stokes equations for a two-phase flow lead, under certain simplifying assumptions [5], to a porous 6 equations system composed of :

Mass equations for the liquid and vapor phases

$$\phi\frac{\partial\alpha_v\rho_v}{\partial t}+\vec{\nabla}(\phi\alpha_v\rho_v\vec{V_v})=\phi\Gamma_v \tag{I.1}$$

$$\phi\frac{\partial\alpha_l\rho_l}{\partial t}+\vec{\nabla}(\phi\alpha_l\rho_l\vec{V_l})=-\phi\Gamma_v \tag{I.2}$$

Momentum equations for the liquid and vapor phases

$$\phi\frac{\partial(\alpha_l\rho_l\vec{V_l})}{\partial t}+\nabla.(\phi\alpha_l\rho_l\vec{V_l}\otimes\vec{V_l})+\nabla.(\phi\alpha_l\rho_l\bar{\bar{D}}\vec{V_l})+\phi\alpha_l\nabla P=\nabla.(\bar{\bar{\sigma}}_l)+\phi P\nabla\alpha_l-\phi F_i+\phi\tau_l+\phi\alpha_l\rho_l\vec{g} \tag{I.3}$$

$$\phi\frac{\partial(\alpha_v\rho_v\vec{V_v})}{\partial t}+\nabla.(\phi\alpha_v\rho_v\vec{V_v}\otimes\vec{V_v})+\nabla.(\phi\alpha_v\rho_v\bar{\bar{D}}\vec{V_v})+\phi\alpha_v\nabla P=\nabla.(\bar{\bar{\sigma}}_v)+\phi P\nabla\alpha_v+\phi F_i+\phi\tau_v+\phi\alpha_v\rho_v\vec{g} \tag{I.4}$$

Total energy equations for the liquid and the vapor phases

$$\phi\frac{\partial(\alpha_l\rho_lE_l)}{\partial t}+\nabla.(\phi\alpha_l\rho_lH_l\vec{V_l})+\phi P\frac{\partial(\alpha_l)}{\partial t}+\nabla.(\phi\alpha_l\rho_lDH_l)=\nabla.(q_l)+\phi\alpha_l\rho_l\vec{g}\vec{V_l}+\phi Q_l+\phi\Gamma_l^E \tag{I.5}$$

$$\phi\frac{\partial(\alpha_v\rho_v E_v)}{\partial t}+\nabla.(\phi\alpha_v\rho_v H_v\vec{V_v})+\phi P\frac{\partial(\alpha_v)}{\partial t}+\nabla.(\phi\alpha_v\rho_v DH_v) = \nabla.(q_v)+\phi\alpha_v\rho_v\vec{g}\vec{V_v}+\phi Q_v+\phi\Gamma_v^E \quad \text{(I.6)}$$

I.2 Porous 4 equations model

The porous 4 equations model is a deduction of the 6 equations model (see section I.1) and is composed of:

- Mixture mass conservation equation;
- Vapor mass balance equation;
- Mixture momentum conservation equation;
- Mixture internal energy balance equation.

To this system will be added two algebraic equations. One that describes the relative velocity and the other the thermodynamic disequilibrium. The relative velocity is obtained using a table or through a drift model. To determine the thermodynamic disequilibrium we assume that one the phases is at at saturation state(here the vapor phase is considered to be at saturation).

I.2.1 Mixture mass conservation equation

The operators that occur in the liquid mass equation(I.2) and the vapor mass equation (I.1) are all linear. Thus, by summing these two balance equations, we easily obtain a mixture mass conservation equation:

$$\phi\frac{\partial\rho}{\partial t}+\nabla.(\phi\rho\vec{V}) = 0 \quad \text{(I.7)}$$

I.2.2 Vapor mass balance equation

Let us begin by recalling the definition of the mixture relative velocity :

$$\vec{V_r} = \vec{V_v} - \vec{V_l} \quad \text{(I.8)}$$

$$\Rightarrow \begin{cases} \vec{V_v} = \vec{V} + (1-C)\vec{V_r} \\ \vec{V_l} = \vec{V} - C\vec{V_r} \end{cases} \quad \text{(I.9)}$$

This will allow us to rewrite the vapor mass balance equation (I.1) where only the the mixture variables should appear:

$$\phi\frac{\partial(\rho C)}{\partial t}+\nabla.(\phi\rho C\vec{V})+\nabla.(\phi\rho(C(1-C)\vec{V_r})=\phi\Gamma_v \tag{I.10}$$

I.2.3 Mixture momentum conservation equation

The mixture momentum conservation equation is obtained by summing the liquid momentum equation (I.3) and the vapor momentum equation (I.4).

The terms that describe the inter-facial exchange in the two equations cancel each other. Besides, we neglect without justification (as in CATHARE and FLICA4) the dispersive terms in each phase(In [5] we propose another approach).
As a result, the mixture momentum equation is written as:

$$\phi\frac{\partial(\rho\vec{V})}{\partial t}+\nabla.(\phi\rho\vec{V}\otimes\vec{V})+\nabla.(\phi\rho C(1-C)\vec{V_r}\otimes\vec{V_r})+\phi\nabla P=\nabla.(\bar{\bar{\sigma}})+\phi\tau+\phi\rho\vec{g} \tag{I.11}$$

which is equivalent(non-conservative form) to:

$$\phi\rho(\frac{\partial\vec{V}}{\partial t}+\vec{V}\nabla.\vec{V})+\nabla.(\phi\rho C(1-C)\vec{V_r}\otimes\vec{V_r})+\phi\nabla P=\nabla.(\bar{\bar{\sigma}})+\phi\tau+\phi\rho\vec{g} \tag{I.12}$$

In this project we make the choice of neglecting the diffusion term. Then the momentum equation (I.12) becomes:

$$\phi\rho(\frac{\partial\vec{V}}{\partial t}+\vec{V}\nabla.\vec{V})+\nabla.(\phi\rho C(1-C)\vec{V_r}\otimes\vec{V_r})+\phi\nabla P=\phi\tau+\phi\rho\vec{g} \tag{I.13}$$

I.2.4 Mixture internal energy balance equation

The mixture internal energy equation is obtained following the same approach as for the momentum equation (I.12), using the liquid internal energy equation (I.5) and the vapor internal energy equation (I.6). This gives us:

$$\phi\frac{\partial\rho E}{\partial t}+\nabla.(\phi\rho H\vec{V})+\nabla.(\phi\rho C(1-C)(H_v-H_l)\vec{V_r})=\phi\rho\vec{g}\vec{V}+\phi Q+\nabla.(q) \tag{I.14}$$

In this project we choose to neglect q which represent the heat flux induced by the thermal conductivity and the turbulent mixing. As a result equation (I.14) becomes:

$$\phi\frac{\partial\rho E}{\partial t}+\nabla.(\phi\rho H\vec{V})+\nabla.(\phi\rho C(1-C)(H_v-H_l)\vec{V_r})=\phi\rho\vec{g}\vec{V}+\phi Q \tag{I.15}$$

Using the relation $H = E + \frac{P}{\rho}$, the equation (I.15) is equivalent to:

$$\phi\frac{\partial \rho E}{\partial t} + \nabla.(\phi\rho E\vec{V}) + \nabla.(\phi P\vec{V}) + \nabla.(\phi\rho C(1-C)(H_v - H_l)\vec{V_r}) = \phi\rho\vec{g}\vec{V} + \phi Q \tag{I.16}$$

Next we multiply the mixture momentum equation (I.11) by $\vec{V}$. We get the kinetic energy evolution:

$$\phi\frac{\partial(\frac{1}{2}\rho\vec{V}^2)}{\partial t} + \nabla.(\phi\rho\frac{1}{2}\vec{V}^2\vec{V}) + \nabla.(\phi\rho C(1-C)\vec{V_r}\otimes\vec{V_r})\vec{V} + \phi\vec{V}\nabla P = \phi\tau\vec{V} + \phi\rho\vec{g}\vec{V} \tag{I.17}$$

According to the relation $E = e + \frac{1}{2}\vec{V}^2$, we obtain the mixture internal energy equation as a difference between the kinetic energy evolution (I.17) and the total energy equation (I.16):

$$\phi\frac{\partial(\rho e)}{\partial t} + \nabla.(\phi\rho e\vec{V}) + P\nabla.(\phi\vec{V}) + \nabla.(\phi\rho C(1-C)(H_v - H_l)\vec{V_r}) - \nabla.(\phi\rho C(1-C)\vec{V_r}\otimes\vec{V_r})\vec{V} = \phi Q - \phi\tau\vec{V}$$

We neglect without justification the terms $\nabla.(\phi\rho C(1-C)\vec{V_r}\otimes\vec{V_r})\vec{V}$ and $\phi\tau\vec{V}$.

Finally, the mixture internal energy equation is given by:

$$\phi\frac{\partial(\rho e)}{\partial t} + \nabla.(\phi\rho e\vec{V}) + P\nabla.(\phi\vec{V}) + \nabla.(\phi\rho C(1-C)(H_v - H_l)\vec{V_r}) = \phi Q \tag{I.18}$$

I.2.5 Closure laws

Thermodynamic disequilibrium

The 4 equations that we have seen in the last section need to be completed by state laws. When the vapor phase is at thermodynamic disequilibrium the vapor enthalpy is a function of vapor density and pressure:

$$h_v = h_v(\rho_v, P)$$

Besides, In FLICA4 we assume one of the phases to be at saturation. In this case the vapor density and the pressure are no longer independents. Then we have:

$$\rho_v = \rho_{v,sat}(P) \quad \Rightarrow \quad h_v = h_{v,sat}(P)$$

Relative velocity

$$\vec{V_v} - \vec{V_l} = \vec{V_r}(\vec{V}, e, C, P)$$

The computation of the relative velocity will be detailed later.

These laws replace:

- A vapor momentum equation;
- A vapor energy equation.

I.2.6 Source terms of the balance equations

In this section we introduce the source terms that occur in the balance equations and involve specific physical modeling [1].

- Vapor mass equation

In the vapor mass equation (I.10), the source term Γ_v represents the cumulative effects due to vaporization through contact with the heating wall Γ_{wv} and the mass exchange at the interface between phases Γ_{lv}:

$$\Gamma_v = \Gamma_{wv} + \Gamma_{lv} \tag{I.19}$$

- Momentum equation

- **Friction forces**

  The source term τ represent the friction(or charge loss) forces exerted on the mixture by the wall(regular charge loss) τ_w as well as eventual obstructions(singular charge loss) τ_s:

$$\tau = \tau_w + \tau_s \tag{I.20}$$

  – *Regular charge loss*

  It is modeled by :

$$-(\frac{1}{2D_h})\rho\bar{\bar{\Lambda}}_w\overrightarrow{V}\|\overrightarrow{V}\| \tag{I.21}$$

  Where $\bar{\bar{\Lambda}}_w$ is a diagonal tensor:

$$\bar{\bar{\Lambda}}_w = \begin{pmatrix} f_w^x & 0 & 0 \\ 0 & f_w^y & 0 \\ 0 & 0 & f_w^z \end{pmatrix}$$

  The coefficients on the diagonal are a priori not equal depending on each space direction. They model the charge loss distribution in the flow and are obtained using

specific correlations. To simplify the calculations we assume the three coefficients to be constants.

– *singular charge loss*

It is modeled by :

$$-(\frac{K}{2})\rho'\overrightarrow{V}\|\overrightarrow{V}\|1_{z=z_s} \tag{I.22}$$

Where K is a given charge loss coefficient.

It is important to notice that naturally the tensor $\bar{\bar{\mathbb{K}}}$ is anti-symmetric with extra diagonal elements that model the rotating effects because of the mixture grids. We chose a diagonal tensor only to simplify the calculations. And for the same reason, we consider the singular charge loss model to be homogeneous:

$$\rho' = \rho$$

- Internal energy equation

- **Energy sources**

The source term Q represent the energy source injected in the fluid. It is written as a "power density" and/or an "implicit thermal flux" between the heating wall and the fluid. To simplify the calculations we consider only the former type of energy(power density which is given by the user).

I.2.7 Specific coorelations

Vapor mass sources

- **Correlation on overheating**

The source term of vaporization at the wall is given by:

$$\Gamma_{wv} = \frac{\chi\Phi}{\mathbb{L}}\frac{4}{D_{ch}} \tag{I.23}$$

The vaporization flux is calculated as follow:

– when nucleate boiling is saturated $T_{sat} - T_l < 10^{-4} : \chi = 1$

– when nucleate boiling is under-saturated $T_w - T_{sat} > \Delta T_{sat} : \chi = \frac{T_w - T_{sat} - \Delta T_{sat}}{T_w - T_l - \Delta T_{sat}}$

– when nucleate boiling is not reached $T_w - T_{sat} < \Delta T_{sat} : \chi = 0$

- **Correlation on mass exchange between phases**

  The mass exchange between phases depends on an exchange volume density Φ_{lv} at the interface between phases and on the phase change energy:

$$\Gamma_{lv} = \frac{\Phi_{lv}}{h_v - h_l} \tag{I.24}$$

  To simplify the calculations we chose a simple mass exchange model between phases:

$$\Phi_{lv} = \begin{cases} \Phi & if \quad h_{l,sat}(P) \leq h < h_{v,sat}(P) \quad \&\& \quad C < 1 \\ 0 & otherwise \end{cases}$$

  Where Φ is assumed constant in time and space and fixed by the user.

  The phase change can appear only when the mixture enthalpy h is between the liquid enthalpy at saturation and the vapor enthalpy at saturation(two-phase region).

Relative velocity

The relative velocity allows us to efficiently make use of the difference between liquid and vapor velocities while only one momentum equation is used.

In this project, we tested two different correlations on the relative velocity:

- A first one, quite simple, where vapor velocity and liquid velocity are proportionals(slip model):

$$\overrightarrow{V_v} = \gamma \overrightarrow{V_l}\,, \quad \gamma > 0$$

  In this case, the relative velocity can be written as:

$$\overrightarrow{V_r} = \overrightarrow{V}_v - \overrightarrow{V}_l = \frac{\gamma - 1}{1 + C(\gamma - 1)} \overrightarrow{V} \tag{I.25}$$

  To simplify the calculations γ is assumed constant and given by the user.

- The second correlation uses the Drift model of Ishii (see ??????) .

  In this case the relative velocity can be written as ::

$$V_r = \frac{(C_0 - 1)V + V_{v,lim}}{1 - C + C_0(C - \alpha)}$$

  C_0 is a distribution parameter that adjusts the mixture velocity. $V_{v,lim}$ is the vapor velocity limit. C_0 and $V_{v,lim}$ depend on the topology of the flow:

– *in a bubbling flow:*

$$(C_0)_{bubble} = \left(C_{inf} + (1 - C_{inf})\sqrt{\frac{\rho_v}{\rho_l}}\right)\left(1 - e^{-18\alpha}\right)$$

$$(V_{v,lim})_{bubble} = C_l \left(\frac{(\rho_v - \rho_l)\, g\, \sigma}{\rho_l^2}\right)^{1/4} (1-\alpha)^{7/4}$$

– *in an annular-film flow:*

$$B = \frac{\sqrt{1 + 75(1-\alpha)}}{\sqrt{\alpha} + 10^{-3}}$$

$$(C_0)_{annular} = \frac{(1 + B\sqrt{\frac{\rho_v}{\rho_l}})}{(\alpha + B\sqrt{\frac{\rho_v}{\rho_l}})}$$

$$(V_{v,lim})_{annular} = \frac{(1-\alpha)^{3/2}}{\alpha + B\sqrt{\frac{\rho_v}{\rho_l}}} \sqrt{\frac{g\, D_h\, (\rho_v - \rho_l)}{0.015\, \rho_l}}$$

– *and to ensure continuity between the two flows:*

$$C_0 = \frac{(C_0)_{annular}\, (C_0)_{bubble}}{\left((C_0)^{50}_{annular} + (C_0)^{50}_{bubble}\right)^{1/50}}$$

$$V_{v,lim} = \frac{(V_{v,lim})_{bubble}\, (V_{v,lim})_{bubble}}{\left((V_{v,lim})^{8}_{annular} + (V_{v,lim})^{8}_{bulles}\right)^{1/8}}$$

σ denotes the surface tension (in $N.M^{-1}$).
C_{inf} and C_l are adjustable parameters that depend on the geometry of the problem. They are given by:

- for a tube bundle flow: $C_{inf} = 1.32$ and $C_l = 4.5$
- for a rectangular cross section flow $C_{inf} = 1.35$ and $C_l = \sqrt{2}$
- for a circular cross section flow $C_{inf} = 1.2$ and $C_l = \sqrt{2}$

I.2.8 Summary

In section (I.2) we have seen how to pass , from the 6 equations porous model obtained thanks to different assumptions, to the 4 equations porous model which is used in FLICA4 [5]. Let ($\mathcal{M}$)

denote this model.

$$(\mathcal{M})\begin{cases} \phi\dfrac{\partial\rho}{\partial t}+\nabla\cdot(\phi\rho\overrightarrow{V})=0 \\ \phi\dfrac{\partial(\rho C)}{\partial t}+\nabla\cdot(\phi\rho C\overrightarrow{V})+\nabla\cdot(\phi\rho C(1-C)\overrightarrow{V}_r)=\phi\Gamma_v \\ \phi\rho\left(\dfrac{\partial\overrightarrow{V}}{\partial t}+\overrightarrow{V}\nabla\overrightarrow{V}\right)+\nabla\cdot\left(\phi\rho C(1-C)\overrightarrow{V_r}\otimes\overrightarrow{V_r}\right)+\phi\nabla P=\phi\tau+\phi\rho\overrightarrow{g} \\ \phi\dfrac{\partial(\rho e)}{\partial t}+\nabla\cdot\left(\phi\rho e\overrightarrow{V}\right)+P\nabla\cdot\left(\phi\overrightarrow{V}\right)+\nabla\cdot\left(\phi\rho C(1-C)\left(H_v-H_l\right)\overrightarrow{V_r}\right)=\phi Q \end{cases} \tag{I.26}$$

This system has seven unknowns: density ρ, pressure P, concentration C, internal energy e (or enthalpy h) and the velocity vector $\overrightarrow{V}$ in each space direction. These mixture physical quantities are linked by seven coupled equations:

- an equation of state:
$$\mathcal{E}(P,\rho,h \text{ ou } e)=0\ ; \tag{I.27}$$
- a mixture mass conservation equation;
- a vapor mass balance equation;
- a mixture internal energy conservation equation;
- a mixture momentum conservation equation in each space direction.

In the next section (see chapitre II) we give details of the spatial and temporal discretization of each equation of the model $(\mathcal{M})$.

Chapter II

Spatio-temporal discretization of the 4 equations model

II.1 Staggered grid

The discretization of the velocity field and the other variables (pressure,density,...) is made on staggered cells.

Unlike the co-located discretization type where all the variables are defined at the same geometric positions, each variable is defined on its own grid and a different control volume is associated to each variable.

We call "pressure grid" the grid where are defined all the scalar variables (pressure, density, enthalpy, ...).

The pressure cell and the velocity cells are shifted by half a cell on each space direction as in figure (see figure II.1) where the scalar variables are given on the center of the pressure cell while the velocity components on the center of its surface.

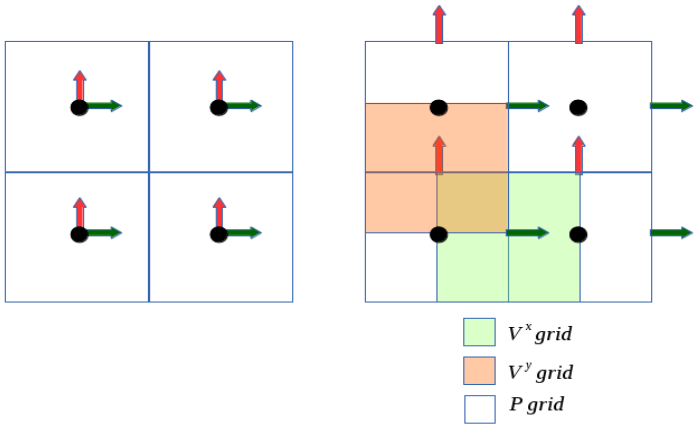

Fig. II.1 : Left side: co-located cells // Right side: staggered cells

Actually the staggered cells(very common in the Navier-stokes equations studies) are very useful despite that they are more difficult to use than the co-located cells.
Indeed, since the pressure cell and the velocity cell are shifted it makes it easier to compute the divergence of the velocity field on the pressure nodes and to avoid the oscillations that we(almost always) get with co-located cells for the low Mach number flows.

The following notations allow a better comprehension of the equations discretization detailed in the next sections. Let us denote by:

- M_c : the pressure cell (cell corresponding to scalar variables);
- M_u : the velocity first component cell (M_c and M_u are shifted by half a cell in the direction of $\vec{e_x}$);
- M_v : the velocity second component cell (M_c and M_v are shifted by half a cell in the direction of $\vec{e_y}$);
- M_w : the velocity third component cell (M_c and M_w are shifted by half a cell in the direction of $\vec{e_z}$);
- σ : the common interface between two neighboring cells M^K and M^L;

$\forall\, K, \quad \forall\, M_c^K$, we denote by:

- M_c^{Lx} its neighboring cell in the direction of $\vec{e_x}$;
- M_c^{Ly} its neighboring cell in the direction of $\vec{e_y}$;
- M_c^{Lz} its neighboring cell in the direction of $\vec{e_z}$;
- M_c^{Lxy} the neighboring cell of M_c^{Lx} in the direction of $\vec{e_y}$;
- M_c^{Lxz} the neighboring cell of M_c^{Lx} in the direction of $\vec{e_z}$;
- M_c^{+Lx} the neighboring cell of M_c^K in the direction of $(+\vec{e}_x)$;
- M_c^{-Lx} the neighboring cell of M_c^K in the direction of $(-\vec{e}_x)$;
- M_c^{+Ly} the neighboring cell of M_c^K in the direction of $(+\vec{e}_y)$;
- M_c^{-Ly} the neighboring cell of M_c^K in the direction of $(-\vec{e}_y)$;
- M_c^{+Lz} the neighboring cell of M_c^K in the direction of $(+\vec{e}_z)$;
- M_c^{-Lz} the neighboring cell of M_c^K in the direction of $(-\vec{e}_z)$;
- M_c^{++Lxy} the neighboring cell of M_c^{+Lx} in the direction of $(+\vec{e}_y)$;

- M_c^{-+Lxy} the neighboring cell of M_c^{-Lx} in the direction of $(+\vec{e}_y)$;
- M_c^{--Lxy} the neighboring cell of M_c^{-Lx} in the direction of $(-\vec{e}_y)$;
- ϵ_K the set of faces of M_c^K;
- $\vec{n}_\sigma$ the outward normal vector to the surface σ;
- $\mathbb{S}_\sigma$ crossing surface of σ (product of its surface by porosity).

II.2 Discretization of the mixture mass equation

The temporal discretization of the mixture mass equation that we try to solve is based on a "semi-implicit" scheme. More precisely, the mass and density fluxes are approximated on the interface using an upwind semi-implicit scheme where the velocity is being implicit while the scalar variables are explicit.

This approach seems necessary when we use a solving method like "solveur de pression" ????? (see chapter III) where variables are implicit only on their own cell. In this way the size of the matrix to inverse will be smaller and the resolution easier.

The spatial discretization of the convection term in the mixture mass equation is done by approximating the density on the cell faces by using an upwind semi-implicit scheme, similarly in the three directions.

The finite volumes discretization of the mixture mass equation involves its integration in time between t_n and t_{n+1} and in space on an elementary control volume M_c^K (or $\mathbb{V}_{M_c^K}$)

$$\int_{M_c^K}\int_{t_n}^{t_{n+1}} (\phi\frac{\partial\rho}{\partial t} + \nabla.(\phi\rho\vec{V}))\,\mathrm{d}\Omega\mathrm{d}t = 0 \tag{II.1}$$

By using the divergence theorem the equation (II.1) becomes:

$$\int_{M_c^K}\int_{t_n}^{t_{n+1}} \phi\frac{\partial\rho}{\partial t}\,\mathrm{d}\Omega\mathrm{d}t + \int_{\mathrm{d}M_c^K}\int_{t_n}^{t_{n+1}} \phi\rho\vec{V}\mathrm{d}S.\vec{n}\,\mathrm{d}t = 0 \tag{II.2}$$

or in discrete form:

$$\mathbb{V}_{M_c^K}(\rho_{M_c^K}^{n+1} - \rho_{M_c^K}^{n}) + \Delta t\sum_{\sigma\in\varepsilon_K}\mathbb{S}_\sigma(\rho^D)_\sigma^n\vec{V}_\sigma^{n+1}.\vec{n}_\sigma = 0 \tag{II.3}$$

$$\Rightarrow \frac{\rho_{M_c^K}^{n+1} - \rho_{M_c^K}^{n}}{\Delta t} + \frac{1}{\mathbb{V}_{M_c^K}}\sum_{\sigma\in\varepsilon_K}\mathscr{F}_\sigma^{n+1} = 0 \tag{II.4}$$

$\mathscr{F}_\sigma^{n+1}$ represents the flux approximation on the interface σ at time t_{n+1}.

To establish the discrete mass equation, all we need now is to approximate the flux $\mathscr{F}_\sigma^{n+1}$ on the 6 faces of a given cell M_c^K. To ensure the stability of the numerical scheme, we use an upwind approximation of the convection term:

$$\mathscr{F}_\sigma^{n+1} = \mathbb{S}_\sigma(\rho^D)_\sigma^n\vec{V}_\sigma^{n+1}.\vec{n}_\sigma \tag{II.5}$$

Here $(\rho^D)_\sigma^n$ represents the mixture density on the interface σ between a given cell M_c^K and a neighboring cell M_c^L.

$$(\rho^D)^n_\sigma = \begin{cases} \rho^n_{M_c^K} \text{ if } & \vec{V}^{n+1}_\sigma.\vec{n}_\sigma > 0 \\ \rho^n_{M_c^L} \text{ otherwise} & \end{cases}$$

As a result, the discrete form of the mixture mass equation (II.4) can be written as:

$$F^1(\rho^{n+1}_{M_c^K}, V^{n+1}_{\sigma\in\epsilon_K}) = 0 \tag{II.6}$$

Taking into account the state equation (I.27), the equation (II.6) becomes:

$$F^1(P^{n+1}_{M_c^K}, h^{n+1}_{M_c^K}, V^{n+1}_{\sigma\epsilon_K}) = 0 \tag{II.7}$$

Finally we compute the derivatives of F^1 (II.7) with respect to each of its variables:

$$\begin{cases} \frac{\partial F^1}{\partial P^{n+1}_{M_c^K}} = \frac{1}{\Delta t}\frac{\partial \rho^{n+1}_{M_c^K}}{\partial P^{n+1}_{M_c^K}} \\ \\ \frac{F^1}{\partial h^{n+1}_{M_c^K}} = \frac{1}{\Delta t}\frac{\partial \rho^{n+1}_{M_c^K}}{\partial h^{n+1}_{M_c^K}} \\ \\ \frac{F^1}{\partial V^{n+1}_{\sigma\in\epsilon_K}} = sign(\vec{n}_\sigma.\vec{e})\frac{\mathbb{S}_\sigma(\rho^D)^n_\sigma}{\mathbb{V}_{M_c^K}} \end{cases}$$

Where:

$$\vec{e} \in \{\vec{e_x}, \vec{e_y}, \vec{e_z}\}$$

$$\vec{V}_\sigma \in \left\{\vec{V}_{M_u^K}, \vec{V}_{M_u^{-Lx}}, \vec{V}_{M_v^K}, \vec{V}_{M_v^{-Ly}}, \vec{V}_{M_w^K}, \vec{V}_{M_w^{-Lz}}\right\}$$

II.3 Discretization of the vapor mass equation

The spatial and temporal discretization of the vapor mass balance equation is done exactly the same way as for the mixture mass equation.

We integrate the vapor mass equation between the time instants t_n and t_{n+1} on the cell M_c^K:

$$\int_{M_c^K}\int_{t_n}^{t_{n+1}} (\phi\frac{\partial \rho C}{\partial t} + \nabla.(\phi\rho C\vec{V}) + \nabla.(\phi\rho C(1-C)\vec{V}_r) - \phi\Gamma_v)\,\mathrm{d}\Omega\mathrm{d}t = 0 \tag{II.8}$$

$$\Rightarrow \frac{(\rho C)^{n+1}_{M_c^K} - (\rho C)^n_{M_c^K}}{\Delta t} + \frac{1}{\mathbb{V}_{M_c^K}}\sum_{\sigma\in\epsilon_K}\left[\mathscr{F}_\sigma^{n+1} + \mathscr{G}_\sigma^{n+1}\right] - (\Gamma_v)^n_{M_c^K} = 0 \tag{II.9}$$

Where:

$$\mathscr{F}_\sigma^{n+1} = \mathbb{S}_\sigma[(\rho C)^D]^n_\sigma \vec{V}_\sigma^{n+1}.\vec{n}_\sigma$$

$$\mathscr{G}_\sigma^{n+1} = \mathbb{S}_\sigma[(\rho_r C_r(1-C_r))^D]^n_\sigma (\vec{V}_r)_\sigma^{n+1}.\vec{n}_\sigma$$

- $\mathscr{F}_\sigma^{n+1}$ and $\mathscr{G}_\sigma^{n+1}$ are the approximations of the fluxes on the interface σ at time t_{n+1};
- $(\vec{V}_r)_\sigma^{n+1}$ is the relative velocity which is given (see I.25) by:
  - Using the slip model: $(\vec{V}_r)_\sigma^{n+1} = \frac{\gamma-1}{1+C_\sigma^n(\gamma-1)}\vec{V}_\sigma^{n+1}$
  - Using the Ishii model: $(\vec{V}_r)_\sigma^{n+1} = \frac{(C_0-1)\vec{V}_\sigma^{n+1}+\vec{V}_{v,lim}}{1-C_\sigma^n+C_0(C_\sigma^n-\alpha_\sigma^n)}$
- C_σ^n, $(\rho C)_\sigma^n$ and $(\rho_r C_r(1-C_r))_\sigma^n$ are defined only at the cells center. On the faces they are approximated using the following upwind scheme:

$$C_\sigma^n = \begin{cases} C^n_{\mathscr{M}_c^K} \text{ if } \quad \vec{V}_\sigma^{n+1}.\vec{n}_\sigma > 0 \\ C^n_{\mathscr{M}_c^L} \text{ otherwise} \end{cases} \tag{II.10}$$

$$(\rho C)_\sigma^n = \begin{cases} (\rho C)^n_{\mathscr{M}_c^K} \text{ if } \quad \vec{V}_\sigma^{n+1}.\vec{n}_\sigma > 0 \\ (\rho C)^n_{\mathscr{M}_c^L} \text{ otherwise} \end{cases} \tag{II.11}$$

$$[(\rho_r C_r(1-C_r))^D]^n_\sigma = \begin{cases} (\rho C(1-C))^n_{\mathscr{M}_c^K} \text{ if } \quad (\vec{V}_r)_\sigma^{n+1}.\vec{n}_\sigma > 0 \\ (\rho C(1-C))^n_{\mathscr{M}_c^L} \text{ otherwise} \end{cases} \tag{II.12}$$

As a result, the discrete form of the vapor mass equation (II.9) can be written as:

$$F^2(\rho^{n+1}_{\mathscr{M}_c^K}, C^{n+1}_{\mathscr{M}_c^K}, V^{n+1}_{\sigma\in\epsilon_K}, (V_r)^{n+1}_{\sigma\in\epsilon_K}) = 0 \tag{II.13}$$

Taking into account the state equation (I.27), the equation (II.13) becomes:

$$F^2(P^{n+1}_{\mathscr{M}_c^K}, h^{n+1}_{\mathscr{M}_c^K}, C^{n+1}_{\mathscr{M}_c^K}, V^{n+1}_{\sigma\in\epsilon_K}) = 0 \tag{II.14}$$

Finally we compute the derivatives of F^2 (II.14) with respect to each of its variables:

$$\begin{cases} \frac{\partial F^2}{\partial P^{n+1}_{M_c^K}} = \frac{C^{n+1}_{\mathscr{M}_c^K}}{\Delta t}\frac{\partial \rho^{n+1}_{M_c^K}}{\partial P^{n+1}_{M_c^K}} \\ \\ \frac{F^2}{\partial h^{n+1}_{M_c^K}} = \frac{C^{n+1}_{\mathscr{M}_c^K}}{\Delta t}\frac{\partial \rho^{n+1}_{M_c^K}}{\partial h^{n+1}_{M_c^K}} \\ \\ \frac{\partial F^2}{\partial C^{n+1}_{\mathscr{M}_c^K}} = \frac{\rho^{n+1}_{\mathscr{M}_c^K}}{\Delta t} \\ \\ \frac{F^2}{\partial V^{n+1}_{\sigma\in\epsilon_K}} = sign(\vec{n}_\sigma.\vec{e})\frac{\mathbb{S}_\sigma}{\mathbb{V}_{M_c^K}}[\rho C - (\rho_r C_r(1-C_r))^n_\sigma \frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_{\sigma\in\epsilon_K}}] \end{cases}$$

where :

- Using the slip model: $\frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} = \frac{\gamma-1}{1+C^n_\sigma(\gamma-1)}$
- Using the Ishii model: $\frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} = \frac{(C_0-1)}{1-C^n_\sigma+C_0\,(C^n_\sigma-\alpha^n_\sigma)}$

$$\vec{e} \in \{\vec{e_x}, \vec{e_y}, \vec{e_z}\}$$

$$V_\sigma \in \left\{V_{M_u^K}, V_{M_u^{-Lx}}, V_{M_v^K}, V_{M_v^{-Ly}}, V_{M_w^K}, V_{M_w^{-Lz}}\right\}$$

II.4 Discretization of the mixture internal energy balance equation

The spatial and temporal discretization of the mixture internal energy balance equation is done exactly the same way as for the mixture mass equation.

$$\int_{M_c^K}\int_{t_n}^{t_{n+1}}(\phi\frac{\partial\rho e}{\partial t}+\nabla.(\phi\rho e\vec{V})+P\nabla.(\phi\vec{V})+\nabla.(\phi\rho C(1-C)(H_v-H_l)\vec{V_r})-\phi Q\,\mathrm{d}\Omega\mathrm{d}t=0 \quad \text{(II.15)}$$

$$\Rightarrow\frac{(\rho e)_{M_c^K}^{n+1}-(\rho e)_{M_c^K}^{n}}{\Delta t}+\frac{1}{\mathbb{V}_{M_c^K}}\sum_{\sigma\in\epsilon_K}[\mathscr{F}_\sigma^{n+1}+P_{M_c^K}^{n+1}\mathscr{G}_\sigma^{n+1}+\mathscr{H}_\sigma^{n+1}]-(Q)_{M_c^K}^{n}=0 \quad \text{(II.16)}$$

where:

$$\mathscr{F}_\sigma^{n+1}=\mathbb{S}_\sigma[(\rho e)^D]_\sigma^n\vec{V}_\sigma^{n+1}.\vec{n}_\sigma$$

$$\mathscr{G}_\sigma^{n+1}=\mathbb{S}_\sigma\vec{V}_\sigma^{n+1}.\vec{n}_\sigma$$

$$\mathscr{H}_\sigma^{n+1}=\mathbb{S}_\sigma[(\rho_r C_r(1-C_r)(H_v-H_l))^D]_\sigma^n(\vec{V_r})_\sigma^{n+1}.\vec{n}_\sigma$$

- $\mathscr{F}_\sigma^{n+1}$, $\mathscr{G}_\sigma^{n+1}$ and $\mathscr{H}_\sigma^{n+1}$ are the approximations of the fluxes on the interface σ at time t_{n+1};
- $[(\rho e)^D]_\sigma^n$ et $[(\rho_r C_r(1-C_r)(H_v-H_l))^D]_\sigma^n$ are defined only at the cells center. On the faces they are approximated using the following upwind scheme:

$$[(\rho e)^D]_\sigma^n=\begin{cases}(\rho e)_{\mathscr{M}_c^K}^n \text{ if } \quad \vec{V}_\sigma^{n+1}.\vec{n}_\sigma>0\\ (\rho e)_{\mathscr{M}_c^L}^n \text{ otherwise}\end{cases}$$

$$[(\rho_r C_r(1-C_r)(H_v-H_l))^D]_\sigma^n=\begin{cases}(\rho C(1-C)(H_v-H_l))_{\mathscr{M}_c^K}^n \text{ if } \quad (\vec{V_r})_\sigma^{n+1}.\vec{n}_\sigma>0\\ (\rho C(1-C)(H_v-H_l))_{\mathscr{M}_c^L}^n \text{ otherwise}\end{cases}$$

Hence, the discrete form of the mixture internal energy equation (II.16) can be written as:

$$F^3(\rho_{\mathscr{M}_c^K}^{n+1},e_{\mathscr{M}_c^K}^{n+1},V_{\sigma\in\epsilon_K}^{n+1},(V_r)_{\sigma\in\epsilon_K}^{n+1})=0 \quad \text{(II.17)}$$

Taking into account the state equation (I.27), the equation (II.17) becomes:

$$F^3(P_{\mathscr{M}_c^K}^{n+1},h_{\mathscr{M}_c^K}^{n+1},V_{\sigma\in\epsilon_K}^{n+1})=0 \quad \text{(II.18)}$$

Finally we compute the derivatives of F^3 (II.18) with respect to each of its variables:

$$\frac{\partial F^3}{\partial P^{n+1}_{\mathscr{M}_c^K}} = \frac{1}{\Delta t}\frac{\partial (\rho e)^{n+1}_{\mathscr{M}_c^K}}{\partial P^{n+1}_{\mathscr{M}_c^K}} + sign(\vec{n}_\sigma.\vec{e})\frac{\mathbb{S}_\sigma}{\mathbb{V}_{\mathscr{M}_c^K}}\vec{V}^{n+1}_\sigma.\vec{n}_\sigma$$

$$\frac{\partial F^3}{\partial h^{n+1}_{\mathscr{M}_c^K}} = \frac{1}{\Delta t}\frac{\partial (\rho e)^{n+1}_{\mathscr{M}_c^K}}{\partial h^{n+1}_{\mathscr{M}_c^K}} + sign(\vec{n}_\sigma.\vec{e})\frac{\mathbb{S}_\sigma}{\mathbb{V}_{\mathscr{M}_c^K}}\frac{\partial P^{n+1}_{\mathscr{M}_c^K}}{\partial h^{n+1}_{\mathscr{M}_c^K}}\vec{V}^{n+1}_\sigma.\vec{n}_\sigma$$

$$\frac{\partial F^3}{\partial V^{n+1}_{\sigma\in\epsilon_K}} = sign(\vec{n}_\sigma.\vec{e})\frac{\mathbb{S}_\sigma}{\mathbb{V}_{\mathscr{M}_c^K}}[(\rho e)^n_\sigma + P^{n+1}_{\mathscr{M}_c^K} + (\rho_r C_r(1-C_r)(H_v - H_l))^n_\sigma \frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_{\sigma\in\epsilon_K}}]$$

where :

- Using the slip model: $\frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} = \frac{\gamma-1}{1+C^n_\sigma(\gamma-1)}$
- Using the Ishii model: $\frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} = \frac{(C_0-1)}{1-C^n_\sigma+C_0\,(C^n_\sigma-\alpha^n_\sigma)}$

$$\vec{e} \in \{\vec{e_x}, \vec{e_y}, \vec{e_z}\}$$

$$V_\sigma \in \left\{\vec{V}_{M^K_u}, \vec{V}_{M_u^{-Lx}}, \vec{V}_{M^K_v}, \vec{V}_{M_v^{-Ly}}, \vec{V}_{M^K_w}, \vec{V}_{M_w^{-Lz}}\right\}$$

II.5 Discretization of the mixture momentum conservation equation

The temporal discretization of the momentum equation written under its non-conservative form uses, as for the mixture mass equation, a "semi-implicit" scheme: for a given velocity cell, only velocity field at the cell's center and the pressure field at its faces are implicit. The other variables should be explicit.

The spatial discretization is done as follows:

- Unless otherwise indicated, to evaluate the scalar variables on the faces we use the average of its values at the centers.
- To ensure stability, an upwind scheme is used to compute the gradient of the velocity squared in the convection term.

Because we have $\phi\rho\overrightarrow{V}\cdot\nabla\overrightarrow{V} = \nabla\cdot\left(\phi\rho\overrightarrow{V}\otimes\overrightarrow{V}\right) - \overrightarrow{V}\nabla\cdot\left(\phi\rho\overrightarrow{V}\right)$, the mixture momentum equation (I.13) can be written as:

$$\rho\frac{\partial\vec{V}}{\partial t} + \nabla.(\phi\rho\vec{V}\otimes\vec{V}) - \vec{V}\nabla.(\phi\rho\vec{V}) + \nabla.(\phi\rho C(1-C)\vec{V}_r\otimes\vec{V}_r) + \phi\nabla P = \phi\tau + \phi\rho\vec{g} \qquad \text{(II.19)}$$

Later in this section we will give more details about the spatial and temporal discretization of the equation (II.19) projected in the direction $\vec{e}_x$. The discretization in the directions $\vec{e}_y$ and $\vec{e}_z$, is obtained by analogy.

The projection of equation (II.19) in the direction $\overrightarrow{e_x}$ gives:

$$\phi\rho\frac{\partial V^x}{\partial t} + \nabla.(\phi\rho V^x\vec{V}) - V^x\nabla.(\phi\rho\vec{V}) + \nabla.(\phi\rho C(1-C)V_r^x\vec{V}_r) + \phi\frac{\partial P}{\partial x} = \phi\tau^x + \phi\rho g^x \qquad \text{(II.20)}$$

The finite volumes discretization involves the integration of the equation (II.19) in time between t_n and t_{n+1} and in space on an elementary control volume M_u^K (or $\mathbb{V}_{M_u^K}$)

$$\int_{M_u^K}\int_{t_n}^{t_{n+1}}(\phi\rho\frac{\partial V^x}{\partial t} + \nabla.(\phi\rho V^x\vec{V}) - V^x\nabla.(\phi\rho\vec{V}) + \nabla.(\phi\rho C(1-C)V_r^x\vec{V}_r) + \phi\frac{\partial P}{\partial x} - \phi\tau^x - \phi\rho g^x)\,\mathrm{d}\Omega\mathrm{d}t = 0$$

$$\Rightarrow \rho^n_{M_u^K}\frac{(V^x)^{n+1}_{M_u^K}-(V^x)^n_{M_u^K}}{\Delta t}+\frac{1}{\mathbb{V}_{M_u^K}}\sum_{\sigma\in\varepsilon_K}[\mathscr{F}^{n+1}_\sigma-(V^x)^{n+1}_{M_u^K}\mathscr{G}^{n+1}_\sigma+\mathscr{H}^{n+1}_\sigma]$$
$$+(\mathbb{S}_{M_c^{+Lx}}P^{n+1}_{M_c^{+Lx}}-\mathbb{S}_{M_c^K}P^{n+1}_{M_c^K})-(\tau^x)^{n+1}_{M_u^K}-(\rho g^x)^n_{M_u^K}=0 \qquad \text{(II.21)}$$

where :

$$\mathscr{F}^{n+1}_\sigma=\mathbb{S}_\sigma\rho^n_\sigma(V^x)^{n+1}_\sigma\vec{V}^{n+1}_\sigma.\vec{n}_\sigma \qquad \text{(II.22)}$$

$$\mathscr{G}^{n+1}_\sigma=\mathbb{S}_\sigma\rho^n_\sigma\vec{V}^{n+1}_\sigma.\vec{n}_\sigma \qquad \text{(II.23)}$$

$$\mathscr{H}^{n+1}_\sigma=\mathbb{S}_\sigma(\rho_rC_r(1-C_r))^n_\sigma(V^x_r)^{n+1}_\sigma(\vec{V}_r)^{n+1}_\sigma.\vec{n}_\sigma \qquad \text{(II.24)}$$

- $\mathscr{F}^{n+1}_\sigma$, $\mathscr{G}^{n+1}_\sigma$ and $\mathscr{H}^{n+1}_\sigma$ are the approximations of the fluxes at the interface σ at time t_{n+1}.

Approximation of velocity field at the interfaces of M_u^K:

Interface σ_x:

$$\vec{V_{\sigma_{+x}}}.\vec{n}_{\sigma_{+x}}=V^x_{\sigma_{+x}}=\frac{\vec{V_{M_u^K}}+\vec{V_{M_u^{+Lx}}}}{2}.\vec{n}_{\sigma_{+x}}=\frac{V^x_{M_u^K}+V^x_{M_u^{+Lx}}}{2} \qquad \text{(II.25)}$$

$$\vec{V_{\sigma_{-x}}}.\vec{n}_{\sigma_{-x}}=V^x_{\sigma_{-x}}=\frac{\vec{V_{M_u^K}}+\vec{V_{M_u^{-Lx}}}}{2}.\vec{n}_{\sigma_{-x}}=\frac{V^x_{M_u^K}+V^x_{M_u^{+Lx}}}{2} \qquad \text{(II.26)}$$

$$[(V^x)^{n+1}_{\sigma_{+x}}]^D=\begin{cases}(V^x)^{n+1}_{M_u^K}\text{ if }\vec{V}^{n+1}_{\sigma_{+x}}.\vec{n}_{\sigma_{+x}}>0\\(V^x)^n_{M_u^{+Lx}}\text{ otherwise}\end{cases} \qquad \text{(II.27)}$$

$$[(V^x)^{n+1}_{\sigma_{-x}}]^D=\begin{cases}(V^x)^{n+1}_{M_u^K}\text{ if }\vec{V}^{n+1}_{\sigma_{-x}}.\vec{n}_{\sigma_{-x}}>0\\(V^x)^n_{M_u^{-Lx}}\text{ otherwise}\end{cases} \qquad \text{(II.28)}$$

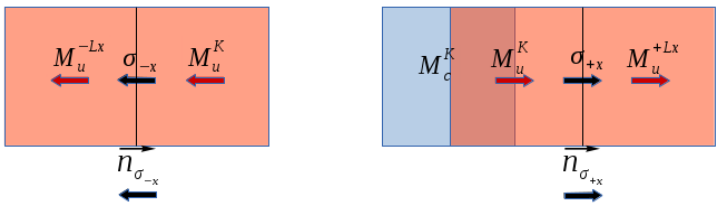

Fig. II.2 : velocity at the interface σ_x of M_u^K

Interface σ_y:

$$\vec{V_{\sigma_{+y}}}.\vec{n}_{\sigma_{+y}} = V^y_{\sigma_{+y}} = \frac{\vec{V_{M_v^K}} + \vec{V_{M_v^{+Lx}}}}{2}.\vec{n}_{\sigma_{+y}} = \frac{V^y_{M_v^K} + V^y_{M_v^{+Lx}}}{2} \tag{II.29}$$

$$[(V^x)^{n+1}_{\sigma_{+y}}]^D = \begin{cases} (V^x)^{n+1}_{M_u^K} \text{ if } \vec{V}^{n+1}_{\sigma_{+y}}.\vec{n}_{\sigma_{+y}} > 0 \\ (V^x)^{n}_{M_u^{+Ly}} \text{ otherwise} \end{cases} \tag{II.30}$$

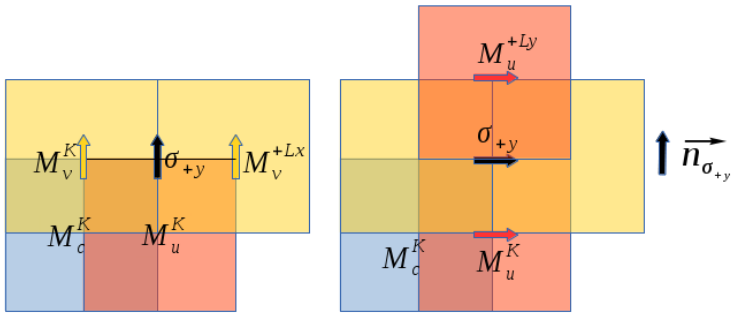

Fig. II.3 : velocity at the interface σ_{+y} de M_u^K

$$\vec{V_{\sigma_{-y}}}.\vec{n}_{\sigma_{-y}} = V^y_{\sigma_{-y}} = \frac{\vec{V_{M_v^{-Ly}}} + \vec{V_{M_v^{+-Lxy}}}}{2}.\vec{n}_{\sigma_{-y}} = \frac{V^y_{M_v^{-Ly}} + V^y_{M_v^{+-Lxy}}}{2} \tag{II.31}$$

$$[(V^x)^{n+1}_{\sigma_{-y}}]^D = \begin{cases} (V^x)^{n+1}_{M_u^K} \text{ if } \vec{V}^{n+1}_{\sigma_{-y}}.\vec{n}_{\sigma_{-y}} > 0 \\ (V^x)^{n}_{M_u^{-Ly}} \text{ otherwise} \end{cases} \tag{II.32}$$

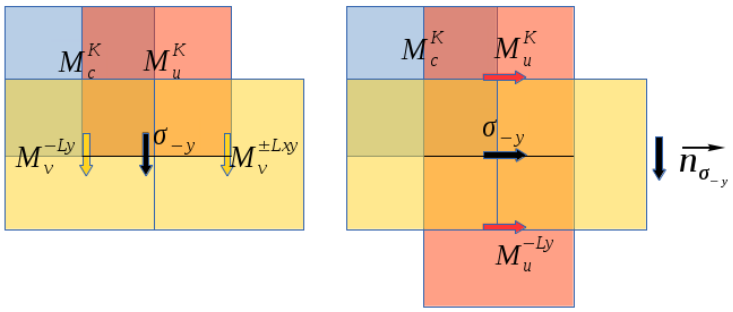

Fig. II.4 : velocity at the interface σ_{-y} de M_u^K

Relative velocity at the interfaces of M_u^K:

- Using the slip model:

$$(\vec{V}_r)^{n+1}_{\sigma} = \frac{\gamma - 1}{1 + C^n_{\sigma}(\gamma - 1)}\vec{V}^{n+1}_{\sigma} \tag{II.33}$$

- Using the Ishii model:

$$(\vec{V}_r)_\sigma^{n+1} = \frac{(C_0 - 1)\vec{V}_\sigma^{n+1} + \vec{V}_{v,lim}}{1 - C_\sigma^n + C_0(C_\sigma^n - \alpha_\sigma^n)} \tag{II.34}$$

$$[(V_r^x)_{\sigma_{+x}}^{n+1}]^D = \begin{cases} (V_r^x)_{M_u^K}^{n+1} \text{ if } (\vec{V}_r)_{\sigma_{+x}}^{n+1}.\vec{n}_{\sigma_{+x}} > 0 \\ (V_r^x)_{M_u^{+Lx}}^{n} \text{ otherwise} \end{cases} \qquad [(V_r^x)_{\sigma_{-x}}^{n+1}]^D = \begin{cases} (V_r^x)_{M_u^K}^{n+1} \text{ if } (\vec{V}_r)_{\sigma_{-x}}^{n+1}.\vec{n}_{\sigma_{-x}} > 0 \\ (V_r^x)_{M_u^{-Lx}}^{n} \text{ otherwise} \end{cases} \tag{II.35}$$

$$[(V_r^x)_{\sigma_{+y}}^{n+1}]^D = \begin{cases} (V_r^x)_{M_u^K}^{n+1} \text{ if } (\vec{V}_r)_{\sigma_{+y}}^{n+1}.\vec{n}_{\sigma_{+y}} > 0 \\ (V_r^x)_{M_u^{+Ly}}^{n} \text{ otherwise} \end{cases} \qquad [(V_r^x)_{\sigma_{-y}}^{n+1}]^D = \begin{cases} (V_r^x)_{M_u^K}^{n+1} \text{ if } (\vec{V}_r)_{\sigma_{-y}}^{n+1}.\vec{n}_{\sigma_{-y}} > 0 \\ (V_r^x)_{M_u^{-Ly}}^{n} \text{ otherwise} \end{cases} \tag{II.36}$$

Approximation of the scalar variables at the interfaces of M_u^K:

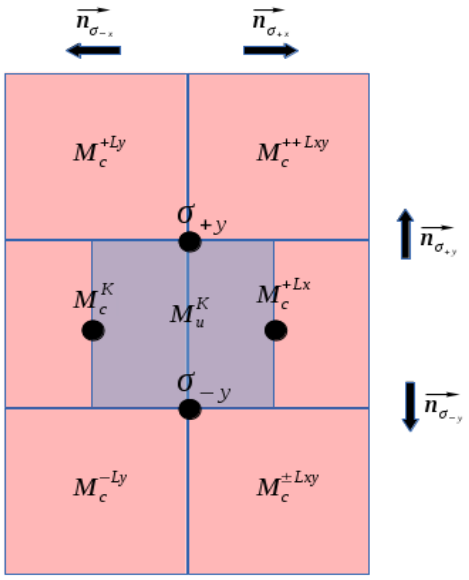

Fig. II.5 : Scalar variables at the interfaces of M_u^K

$$\rho_{M_u^K}^n = \frac{\rho_{M_c^K}^n + \rho_{M_c^{+Lx}}^n}{2}$$

$$\rho_{\sigma_{-x}}^n = \rho_{M_c^K}^n \qquad \rho_{\sigma_{+x}}^n = \rho_{M_c^{+Lx}}^n$$

$$\rho_{\sigma_{+y}}^n = \begin{cases} \frac{\rho_{M_c^K}^n + \rho_{M_c^{+Lx}}^n}{2} \text{ if } \vec{V}_{\sigma_{+y}}^{n+1}.\vec{n}_{\sigma_{+y}} > 0 \\ \frac{\rho_{M_c^{+Ly}}^n + \rho_{M_c^{++Lxy}}^n}{2} \text{ otherwise} \end{cases} \qquad \rho_{\sigma_{-y}}^n = \begin{cases} \frac{\rho_{M_c^K}^n + \rho_{M_c^{+Lx}}^n}{2} \text{ if } \vec{V}_{\sigma_{-y}}^{n+1}.\vec{n}_{\sigma_{-y}} > 0 \\ \frac{\rho_{M_c^{-Ly}}^n + \rho_{M_c^{+-Lxy}}^n}{2} \text{ otherwise} \end{cases}$$

We use the same method to determine $(\rho_r C_r(1-C_r))^n_\sigma$:

$$(\rho_r C_r(1-C_r))^n_{\sigma_{-x}} = (\rho_r C_r(1-C_r))^n_{M_c^K} \qquad (\rho_r C_r(1-C_r))^n_{\sigma_{+x}} = (\rho_r C_r(1-C_r))^n_{M_c^{+Lx}}$$

$$(\rho_r C_r(1-C_r))^n_{\sigma_{+y}} = \begin{cases} \frac{(\rho_r C_r(1-C_r))^n_{M_c^K} + (\rho_r C_r(1-C_r))^n_{M_c^{+Lx}}}{2} & \text{if } (\vec{V_r})^{n+1}_{\sigma_{+y}}.\vec{n}_{\sigma_{+y}} > 0 \\ \frac{(\rho_r C_r(1-C_r))^n_{M_c^{+Ly}} + (\rho_r C_r(1-C_r))^n_{M_c^{++Lxy}}}{2} & \text{otherwise} \end{cases}$$

$$(\rho_r C_r(1-C_r))^n_{\sigma_{-y}} = \begin{cases} \frac{(\rho_r C_r(1-C_r))^n_{M_c^K} + (\rho_r C_r(1-C_r))^n_{M_c^{+Lx}}}{2} & \text{if } (\vec{V_r})^{n+1}_{\sigma_{-y}}.\vec{n}_{\sigma_{-y}} > 0 \\ \frac{(\rho_r C_r(1-C_r))^n_{M_c^{-Ly}} + (\rho_r C_r(1-C_r))^n_{M_c^{+-Lxy}}}{2} & \text{otherwise} \end{cases}$$

NB: At the interfaces σ_{+z} and σ_{-z}, we easily get the same result as at the interfaces σ_{+y} and σ_{-y} if we replace y by z.

Friction forces

We recall (see I.20) that:

$$(\tau^x)^{n+1}_{M_u^K} = (\tau^x_w)^{n+1}_{M_u^K} + (\tau^x_s)^{n+1}_{M_u^K}$$

Then according to (I.21) and (I.22) we have:

$$(\tau^x_w)^{n+1}_{M_u^K} = \frac{-1}{2(D^x_h)_{M_u^K}} \rho^n_{M_u^K} (f^x_w)(V^x)^{n+1}_{M_u^K} |(V^x)^{n+1}_{M_u^K}|$$

$$(\tau^x_s)^{n+1}_{M_u^K} = \frac{-K^x}{2} \rho^n_{M_u^K} (V^x)^{n+1}_{M_u^K} |(V^x)^{n+1}_{M_u^K}|$$

The discretization of the mixture momentum equation in the direction $\vec{e_x}$ (II.21) can be written as:

$$F^4(P^{n+1}_{\mathscr{M}_c^K}, P^{n+1}_{\mathscr{M}_c^{+Lx}}, (V^x)^{n+1}_{\mathscr{M}_u^K}) = 0 \tag{II.37}$$

By analogy, on obtain the discretization in the directions $\vec{e_y}$ and $\vec{e_z}$:

$$F^5(P^{n+1}_{\mathscr{M}_c^K}, P^{n+1}_{\mathscr{M}_c^{+Ly}}, (V^y)^{n+1}_{\mathscr{M}_v^K}) = 0 \tag{II.38}$$

$$F^6(P^{n+1}_{\mathscr{M}_c^K}, P^{n+1}_{\mathscr{M}_c^{+Lz}}, (V^z)^{n+1}_{\mathscr{M}_w^K}) = 0 \tag{II.39}$$

The derivative of F^4 (II.37) are given by:

$$\frac{\partial F^4}{\partial P^{n+1}_{M_c^K}} = -\mathbb{S}_{M_c^K}$$

$$\frac{\partial F^4}{\partial P^{n+1}_{M_c^{+Lx}}} = \mathbb{S}_{M_c^{+Lx}}$$

$$\frac{\partial F^4}{\partial V^{n+1}_{\mathscr{M}_u^K}} = \frac{\rho^n_{\mathscr{M}_u^K}}{\Delta t} + \mathbb{S}_\sigma \rho^n_\sigma ((V^x)^n_\sigma + 1)\, sign(\vec{n}_\sigma.\vec{e}) \frac{\partial \vec{V}^{n+1}_\sigma}{\partial V^{n+1}_{\mathscr{M}_u^K}} +$$
$$\mathbb{S}_\sigma ((\rho_r C_r (1-C_r))^n_\sigma)(V^x)^n_\sigma\, sign(\vec{n}_\sigma.\vec{e}) \frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} \frac{\partial \vec{V}^{n+1}_\sigma}{\partial V^{n+1}_{\mathscr{M}_u^K}} \tag{II.40}$$

According to (II.31), the equation (II.40) becomes:

$$\frac{\partial F^4}{\partial V^{n+1}_{\mathscr{M}_u^K}} = \frac{\rho^n_{\mathscr{M}_u^K}}{\Delta t} + \frac{1}{2}\, \mathbb{S}_\sigma \rho^n_\sigma ((V^x)^n_\sigma + 1)\, sign(\vec{n}_\sigma.\vec{e})$$
$$+\frac{1}{2}\, \mathbb{S}_\sigma ((\rho_r C_r (1-C_r))^n_\sigma)(V^x)^n_\sigma \frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} sign(\vec{n}_\sigma.\vec{e}) \tag{II.41}$$

where:

- Using the slip model: $\frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} = \frac{\gamma - 1}{1 + C^n_\sigma (\gamma - 1)}$
- Using the Ishii model: $\frac{\partial (V_r)^{n+1}_\sigma}{\partial V^{n+1}_\sigma} = \frac{(C_0 - 1)}{1 - C^n_\sigma + C_0\,(C^n_\sigma - \alpha^n_\sigma)}$

By analogy, we determine the derivatives of F^5 and F^6.

Chapter III

Resolution of the 4 equations model

III.1 Construction of the system to solve

Let (S) denote the non linear system we ought to solve at each physical time step:

$$(S)\begin{cases} F^1(P,h,\vec{V})=0 \\ F^2(P,h,C,\vec{V})=0 \\ F^3(P,h,\vec{V})=0 \\ F^4(P,\vec{V})=0 \\ F^5(P,\vec{V})=0 \\ F^6(P,\vec{V})=0 \end{cases} \tag{III.1}$$

To solve this system, we use the Newton-Raphson method:

$$\sum_{j=1}[\frac{\partial F_i}{\partial x_j}]^k.\Delta x_j^{k+1} = -F_i^k \tag{III.2}$$

where :

- F_i^k : residual of the discrete equation i at the iteration k;
- $\Delta x_j^{k+1} = x_j^{k+1} - x_j^k$: increment of the variable x_j at the iteration k;
- $[\frac{\partial F_i}{\partial x_j}]^k$: derivative of the equation i with respect to the variable j at the iteration k.

Let U denote the unknown vector defined by:

$$U = (P,h,C,V^x,V^y,V^z)^t = (P_1,...,P_{N_c},h_1,...,h_{N_c},C_1,...,C_{N_c} \\ ,V_1^x,...,V_{N_x}^x,V_1^y,...,V_{N_y}^y,V_1^z,...,V_{N_z}^z)^t$$

At each iteration of Newton-Raphson, we determine U at the instant t_{n+1} by solving the linear equation $A(U^k)\Delta U^{k+1} = S(U^n, U^k)$:

$$\Leftrightarrow \begin{pmatrix} \frac{\partial F^1}{\partial P} & \frac{\partial F^1}{\partial h} & \frac{\partial F^1}{\partial C} & \frac{\partial F^1}{\partial V^x} & \frac{\partial F^1}{\partial V^y} & \frac{\partial F^1}{\partial V^z} \\ \frac{\partial F^2}{\partial P} & \frac{\partial F^2}{\partial h} & \frac{\partial F^2}{\partial C} & \frac{\partial F^2}{\partial V^x} & \frac{\partial F^2}{\partial V^y} & \frac{\partial F^3}{\partial V^z} \\ \frac{\partial F^3}{\partial P} & \frac{\partial F^3}{\partial h} & \frac{\partial F^3}{\partial C} & \frac{\partial F^3}{\partial V^x} & \frac{\partial F^3}{\partial V^y} & \frac{\partial F^3}{\partial V^z} \\ \frac{\partial F^4}{\partial P} & \frac{\partial F^4}{\partial h} & \frac{\partial F^4}{\partial C} & \frac{\partial F^4}{\partial V^x} & \frac{\partial F^4}{\partial V^y} & \frac{\partial F^4}{\partial V^z} \\ \frac{\partial F^5}{\partial P} & \frac{\partial F^5}{\partial h} & \frac{\partial F^5}{\partial C} & \frac{\partial F^5}{\partial V^x} & \frac{\partial F^5}{\partial V^y} & \frac{\partial F^5}{\partial V^z} \\ \frac{\partial F^6}{\partial P} & \frac{\partial F^6}{\partial h} & \frac{\partial F^6}{\partial C} & \frac{\partial F^6}{\partial V^x} & \frac{\partial F^6}{\partial V^y} & \frac{\partial F^6}{\partial V^z} \end{pmatrix} \begin{pmatrix} \Delta U_1 \\ \Delta U_2 \\ \Delta U_3 \\ \Delta U_4 \\ \Delta U_5 \\ \Delta U_6 \end{pmatrix} = \begin{pmatrix} S^1 = -F^1 \\ S^2 = -F^2 \\ S^3 = -F^3 \\ S^4 = -F^4 \\ S^5 = -F^5 \\ S^6 = -F^6 \end{pmatrix} \tag{III.3}$$

Lets notice that each coefficient of the jacobian $A(U^k)$, whose size is equal to $(3N_c + N_x + N_y + N_z)^2$, is a bloc whose size is equal to:

- $(N_c * N_c)$ for each $\frac{\partial F^i}{\partial \S}$ such as $i \in \{1, 2, 3\}$ and $\S \in \{P, h, C\}$;
- $(N_c * N_e)$ for each $\frac{\partial F^i}{\partial \S}$ such as $i \in \{1, 2, 3\}$ and $(N_e, \S) \in \{(N_x, V^x), (N_y, V^y), (N_z, V^z)\}$;
- $(N_e * N_e)$ for each $\frac{\partial F^i}{\partial \S}$ such as $i \in \{4, 5, 6\}$ and $(N_e, \S) \in \{(N_x, V^x), (N_y, V^y), (N_z, V^z)\}$;
- $(N_e * N_c)$ for each $\frac{\partial F^i}{\partial \S}$ such as $\S \in \{P, h, C\}$ and $(N_e, i) \in \{(N_x, 4), (N_y, 5), (N_z, 6)\}$.

The same applies to the components of ΔU^{k+1} and $S(U^n, U^k)$ which are vectors of size:

- N_c for each $(\Delta U^{k+1})_j$ and S_j such as $j \in \{1, 2, 3\}$;
- N_e for each $(\Delta U^{k+1})_j$ and S_j such as $(j, N_e) \in \{(4, N_x), (5, N_y), (6, N_z)\}$.

To solve the system (III.3) we use and compare two different methods:

* the full Jacobian method (see III.2).

* the "pressure-based solver" method (see III.3).

The two methods are used by CATHARE to solve the 6 equations model. The full Jacobian method is used to deal with the 1D problems since the size of the matrix("not too big") allows it. However in the 2D and 3D problems CATHARE uses the pressure-based method.

III.2 The "full Jacobian" method

This method involves the inversion of the matrix in (III.3) when its size is reasonable. Actually in this case it is very useful since it is simple to implement and because it allows the possibility of "impliciting" all the variables in the discretization step which leads to a better resolution. Despite the efficiency of the full Jacobian method to treat the "small sized" problems, its use is bounded by a limit on the jacobian matrix size. Beyond this limit, the pressure-based method becomes more efficient.

III.3 The "pressure-based solver" method

The "semi-implicit" scheme we used to discretize the 4 equations (see chapter II) allows to simplify significantly the terms of the matrix that occur in the momentum equations F^4, F^5 and F^6. This will enable the expression of the velocity increments as functions of the pressure increments (see section III.3.1) and then to eliminate them. In section (III.3.2) we will see how to eliminate all the scalar variables (but the pressure increments) and then to obtain a linear equation where only the pressure increments should occur.

III.3.1 Elimination of the velocity increments

The purpose of this step is to write the velocity increments as a function of the pressure increments. To do so we consider only the momentum equations which corresponds to this 'partial' linear system:

$$\begin{pmatrix} \frac{\partial F^4}{\partial P} & \frac{\partial F^4}{\partial h} & \frac{\partial F^4}{\partial C} & \frac{\partial F^4}{\partial V^x} & \frac{\partial F^4}{\partial V^y} & \frac{\partial F^4}{\partial V^z} \\ \frac{\partial F^5}{\partial P} & \frac{\partial F^5}{\partial h} & \frac{\partial F^5}{\partial C} & \frac{\partial F^5}{\partial V^x} & \frac{\partial F^5}{\partial V^y} & \frac{\partial F^5}{\partial V^z} \\ \frac{\partial F^6}{\partial P} & \frac{\partial F^6}{\partial h} & \frac{\partial F^6}{\partial C} & \frac{\partial F^6}{\partial V^x} & \frac{\partial F^6}{\partial V^y} & \frac{\partial F^6}{\partial V^z} \end{pmatrix} \begin{pmatrix} \Delta U_1 \\ \Delta U_2 \\ \Delta U_3 \\ \Delta U_4 \\ \Delta U_5 \\ \Delta U_6 \end{pmatrix} = \begin{pmatrix} S^4 \\ S^5 \\ S^6 \end{pmatrix} \tag{III.4}$$

According to (II.37),(II.38) and (II.39), the functions F^4, F^5 and F^6 don't depend on h and C at time step t^{n+1}. Thus their derivatives with respect to these variables are equals to zero as well as:

- the derivative of F^4 with respect to V^y and V^z;
- the derivative of F^5 with respect to V^x and V^z;
- the derivative of F^6 with respect to V^x and V^y.

In this case, the system (III.4) becomes:

$$\begin{pmatrix} \frac{\partial F^4}{\partial P} & 0 & 0 & \frac{\partial F^4}{\partial V^x} & 0 & 0 \\ \frac{\partial F^5}{\partial P} & 0 & 0 & 0 & \frac{\partial F^5}{\partial V^y} & 0 \\ \frac{\partial F^6}{\partial P} & 0 & 0 & 0 & 0 & \frac{\partial F^6}{\partial V^z} \end{pmatrix} \begin{pmatrix} \Delta U_1 \\ \Delta U_2 \\ \Delta U_3 \\ \Delta U_4 \\ \Delta U_5 \\ \Delta U_6 \end{pmatrix} = \begin{pmatrix} S^4 \\ S^5 \\ S^6 \end{pmatrix} \tag{III.5}$$

where:

$$\frac{\partial F^4}{\partial P} = \begin{pmatrix} \frac{\partial F^4_{M_u^0}}{\partial P_{M_c^0}} & \frac{\partial F^4_{M_u^0}}{\partial P_{M_c^{1x}}} & 0 & \dots \\ 0 & \frac{\partial F^4_{M_u^K}}{\partial P_{M_c^K}} & \frac{\partial F^4_{M_u^K}}{\partial P_{M_c^{+Lx}}} & 0 & \dots \\ 0 & \dots & 0 & 0 & \frac{\partial F^4_{M_u^{N_x}}}{\partial P_{M_c^{N_c}}} \end{pmatrix} \frac{\partial F^4}{\partial V^x} = \begin{pmatrix} \frac{\partial F^4_{M_u^0}}{\partial V^x_{M_u^0}} & 0 & \dots & 0 \\ 0 & \frac{\partial F^4_{M_u^K}}{\partial V^x_{M_u^K}} & 0 & \dots \\ 0 & \dots & 0 & \frac{\partial F^4_{M_u^{N_x}}}{\partial V^x_{M_u^{N_x}}} \end{pmatrix}$$

$$\frac{\partial F^5}{\partial P} = \begin{pmatrix} \frac{\partial F^5_{M_v^0}}{\partial P_{M_c^0}} & \frac{\partial F^5_{M_v^0}}{\partial P_{M_c^{1y}}} & 0 & \dots \\ 0 & \frac{\partial F^5_{M_v^K}}{\partial P_{M_c^K}} & \frac{\partial F^5_{M_v^K}}{\partial P_{M_c^{+Ly}}} & 0 & \dots \\ 0 & \dots & 0 & 0 & \frac{\partial F^5_{M_v^{N_y}}}{\partial P_{M_c^{N_c}}} \end{pmatrix} \frac{\partial F^5}{\partial V^y} = \begin{pmatrix} \frac{\partial F^5_{M_v^0}}{\partial V^y_{M_v^0}} & 0 & \dots & 0 \\ 0 & \frac{\partial F^5_{M_v^K}}{\partial V^y_{M_v^K}} & 0 & \dots \\ 0 & \dots & 0 & \frac{\partial F^5_{M_v^{N_y}}}{\partial V^y_{M_v^{N_y}}} \end{pmatrix}$$

$$\frac{\partial F^6}{\partial P} = \begin{pmatrix} \frac{\partial F^6_{M_w^0}}{\partial P_{M_c^0}} & \frac{\partial F^6_{M_w^0}}{\partial P_{M_c^{1z}}} & 0 & \dots \\ 0 & \frac{\partial F^6_{M_w^K}}{\partial P_{M_c^K}} & \frac{\partial F^6_{M_w^K}}{\partial P_{M_c^{+Lz}}} & 0 & \dots \\ 0 & \dots & 0 & 0 & \frac{\partial F^6_{M_w^{N_z}}}{\partial P_{M_c^{N_c}}} \end{pmatrix} \frac{\partial F^6}{\partial V^z} = \begin{pmatrix} \frac{\partial F^6_{M_w^0}}{\partial V^z_{M_w^0}} & 0 & \dots & 0 \\ 0 & \frac{\partial F^6_{M_w^K}}{\partial V^z_{M_w^K}} & 0 & \dots \\ 0 & \dots & 0 & \frac{\partial F^6_{M_w^{N_z}}}{\partial V^z_{M_w^{N_z}}} \end{pmatrix}$$

By developing the equation (III.5) in a cell M_u^K, we obtain the following equation system:

$$\begin{cases} \frac{\partial F^4_{M_u^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} + \frac{\partial F^4_{M_u^K}}{\partial P_{M_c^{+Lx}}}(\Delta P)_{M_c^{+Lx}} + \frac{\partial F^4_{M_u^K}}{\partial V^x_{M_u^K}}(\Delta V^x)_{M_u^K} = S^4_{M_u^K} \\ \frac{\partial F^5_{M_v^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} + \frac{\partial F^5_{M_v^K}}{\partial P_{M_c^{+Ly}}}(\Delta P)_{M_c^{+Ly}} + \frac{\partial F^5_{M_v^K}}{\partial V^y_{M_v^K}}(\Delta V^y)_{M_v^K} = S^5_{M_v^K} \\ \frac{\partial F^6_{M_w^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} + \frac{\partial F^6_{M_w^K}}{\partial P_{M_c^{+Lz}}}(\Delta P)_{M_c^{+Lz}} + \frac{\partial F^6_{M_w^K}}{\partial V^z_{M_w^K}}(\Delta V^z)_{M_w^K} = S^6_{M_w^K} \end{cases} \quad \text{(III.6)}$$

$$\Rightarrow \begin{cases} (\Delta V^x)_{M_u^K} = \frac{1}{\frac{\partial F^4_{M_u^K}}{\partial V^x_{M_u^K}}}[S^4_{M_u^K} - \frac{\partial F^4_{M_u^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} - \frac{\partial F^4_{M_u^K}}{\partial P_{M_c^{+Lx}}}(\Delta P)_{M_c^{+Lx}}] \\ (\Delta V^y)_{M_v^K} = \frac{1}{\frac{\partial F^5_{M_v^K}}{\partial V^y_{M_v^K}}}[S^5_{M_v^K} - \frac{\partial F^5_{M_v^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} - \frac{\partial F^5_{M_v^K}}{\partial P_{M_c^{+Ly}}}(\Delta P)_{M_c^{+Ly}}] \\ (\Delta V^z)_{M_w^K} = \frac{1}{\frac{\partial F^6_{M_w^K}}{\partial V^z_{M_w^K}}}[S^6_{M_w^K} - \frac{\partial F^6_{M_w^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} - \frac{\partial F^6_{M_w^K}}{\partial P_{M_c^{+Lz}}}(\Delta P)_{M_c^{+Lz}}] \end{cases} \quad \text{(III.7)}$$

By analogy we determine the velocity increments $(\Delta V^x)_{M_u^{-Lx}}$, $(\Delta V^y)_{M_v^{-Ly}}$ and $(\Delta V^z)_{M_w^{-Lz}}$ as functions of the pressure increments:

$$\begin{cases} (\Delta V^x)_{M_u^{-Lx}} = \frac{1}{\frac{\partial F^4_{M_u^{-Lx}}}{\partial V^x_{M_u^{-Lx}}}}[S^4_{M_u^{-Lx}} - \frac{\partial F^4_{M_u^{-Lx}}}{\partial P_{M_c^{-Lx}}}(\Delta P)_{M_c^{-Lx}} - \frac{\partial F^4_{M_u^{-Lx}}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K}] \\ (\Delta V^y)_{M_v^{-Ly}} = \frac{1}{\frac{\partial F^5_{M_v^{-Ly}}}{\partial V^y_{M_v^{-Ly}}}}[S^5_{M_v^{-Ly}} - \frac{\partial F^5_{M_v^{-Ly}}}{\partial P_{M_c^{-Ly}}}(\Delta P)_{M_c^{-Ly}} - \frac{\partial F^5_{M_v^{-Ly}}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K}] \\ (\Delta V^z)_{M_w^{-Lz}} = \frac{1}{\frac{\partial F^6_{M_w^{-Lz}}}{\partial V^z_{M_w^{-Lz}}}}[S^6_{M_w^{-Lz}} - \frac{\partial F^6_{M_w^{-Lz}}}{\partial P_{M_c^{-Lz}}}(\Delta P)_{M_c^{-Lz}} - \frac{\partial F^6_{M_w^{-Lz}}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K}] \end{cases} \quad \text{(III.8)}$$

This step enabled the writing of the velocity increments(ΔU_4, ΔU_5 and ΔU_6) at each face of the mesh as functions of the pressure increments. This will be useful in the next step (see section III.3.2) to establish a linear pressure equation (such as only pressure increments are unknown).

III.3.2 Triangulation

In this step we aim to eliminate the scalar variables increments. To do so we use the three scalar variables equations (mass, concentration and energy), which corresponds to the following system:

$$\begin{pmatrix} \frac{\partial F^1}{\partial P} & \frac{\partial F^1}{\partial h} & \frac{\partial F^1}{\partial C} & \frac{\partial F^1}{\partial V^x} & \frac{\partial F^1}{\partial V^y} & \frac{\partial F^1}{\partial V^z} \\ \frac{\partial F^2}{\partial P} & \frac{\partial F^2}{\partial h} & \frac{\partial F^2}{\partial C} & \frac{\partial F^2}{\partial V^x} & \frac{\partial F^2}{\partial V^y} & \frac{\partial F^2}{\partial V^z} \\ \frac{\partial F^3}{\partial P} & \frac{\partial F^3}{\partial h} & \frac{\partial F^3}{\partial C} & \frac{\partial F^3}{\partial V^x} & \frac{\partial F^3}{\partial V^y} & \frac{\partial F^3}{\partial V^z} \end{pmatrix} \begin{pmatrix} \Delta U_1 \\ \Delta U_2 \\ \Delta U_3 \\ \Delta U_4 \\ \Delta U_5 \\ \Delta U_6 \end{pmatrix} = \begin{pmatrix} S^1 \\ S^2 \\ S^3 \end{pmatrix} \tag{III.9}$$

As we did previously, some simplifications take place (thanks to (II.7) and (II.18)) since F^1 and F^3 don't depend on C at t_{n+1}. Thus, the system (III.9) becomes:

$$\begin{pmatrix} \frac{\partial F^1}{\partial P} & \frac{\partial F^1}{\partial h} & 0 & \frac{\partial F^1}{\partial V^x} & \frac{\partial F^1}{\partial V^y} & \frac{\partial F^1}{\partial V^z} \\ \frac{\partial F^2}{\partial P} & \frac{\partial F^2}{\partial h} & \frac{\partial F^2}{\partial C} & \frac{\partial F^2}{\partial V^x} & \frac{\partial F^2}{\partial V^y} & \frac{\partial F^2}{\partial V^z} \\ \frac{\partial F^3}{\partial P} & \frac{\partial F^3}{\partial h} & 0 & \frac{\partial F^3}{\partial V^x} & \frac{\partial F^3}{\partial V^y} & \frac{\partial F^3}{\partial V^z} \end{pmatrix} \begin{pmatrix} \Delta U_1 \\ \Delta U_2 \\ \Delta U_3 \\ \Delta U_4 \\ \Delta U_5 \\ \Delta U_6 \end{pmatrix} = \begin{pmatrix} S^1 \\ S^2 \\ S^3 \end{pmatrix} \tag{III.10}$$

At this stage applying the operations $(L^1) \longleftarrow (L^1) \times \frac{\partial F^2}{\partial h} - (L^3) \times \frac{\partial F^1}{\partial h}$ and then $(L^2) \leftrightarrow (L^3)$ on the system (III.10) results in:

$$\begin{pmatrix} J^{1,1} & 0 & 0 & J^{1,4} & J^{1,5} & J^{1,6} \\ \frac{\partial F^3}{\partial P} & \frac{\partial F^3}{\partial h} & 0 & \frac{\partial F^3}{\partial V^x} & \frac{\partial F^3}{\partial V^y} & \frac{\partial F^3}{\partial V^z} \\ \frac{\partial F^2}{\partial P} & \frac{\partial F^2}{\partial h} & \frac{\partial F^2}{\partial C} & \frac{\partial F^2}{\partial V^x} & \frac{\partial F^2}{\partial V^y} & \frac{\partial F^2}{\partial V^z} \end{pmatrix} \begin{pmatrix} \Delta U_1 \\ \Delta U_2 \\ \Delta U_3 \\ \Delta U_4 \\ \Delta U_5 \\ \Delta U_6 \end{pmatrix} = \begin{pmatrix} D^1 = S^1 \frac{\partial F^2}{\partial h} - S^2 \frac{\partial F^1}{\partial h} \\ S^3 \\ S^2 \end{pmatrix} \tag{III.11}$$

where :

$$J^{1,1}_{M_c^K} = (\frac{\partial F^2_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^1_{M_c^K}}{\partial P_{M_c^K}}) - (\frac{\partial F^1_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^2_{M_c^K}}{\partial P_{M_c^K}})$$

$$J^{1,4}_{M_u^K} = (\frac{\partial F^2_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^1_{M_c^K}}{\partial V^x_{M_u^K}}) - (\frac{\partial F^1_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^2_{M_c^K}}{\partial V^x_{M_u^K}})$$

$$J^{1,5}_{M_v^K} = (\frac{\partial F^2_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^1_{M_c^K}}{\partial V^y_{M_v^K}}) - (\frac{\partial F^1_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^2_{M_c^K}}{\partial V^y_{M_v^K}})$$

$$J^{1,6}_{M_w^K} = \left(\frac{\partial F^2_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^1_{M_c^K}}{\partial V^z_{M_w^K}}\right) - \left(\frac{\partial F^1_{M_c^K}}{\partial h_{M_c^K}} \frac{\partial F^2_{M_c^K}}{\partial V^z_{M_w^K}}\right)$$

We develop the first row of the system (III.11) in a cell M_c^K, we get the following equation:

$$\begin{aligned}(J^{1,1})_{M_c^K}(\Delta P)_{M_c^K} + (J^{1,4})_{M_u^K}(\Delta V^x)_{M_u^K} + (J^{1,4})_{M_u^{-Lx}}(\Delta V^x)_{M_u^{-Lx}} \\ +(J^{1,5})_{M_v^K}(\Delta V^y)_{M_v^K} + (J^{1,5})_{M_v^{-Ly}}(\Delta V^y)_{M_v^{-Ly}} \\ +(J^{1,6})_{M_w^K}(\Delta V^z)_{M_w^K} + (J^{1,6})_{M_w^{-Lz}}(\Delta V^z)_{M_w^{-Lz}} = D^1_{M_c^K}\end{aligned} \tag{III.12}$$

It is at this stage where we make use of the velocity increments we calculated in the last step (see (III.7) and (III.8)). Their integration in the equation (III.12) gives us:

$$\mathbb{A}(\Delta P)_{M_c^K} + \mathbb{B}(\Delta P)_{M_c^{+Lx}} + \mathbb{C}(\Delta P)_{M_c^{-Lx}} + \mathbb{D}(\Delta P)_{M_c^{+Ly}} + \mathbb{E}(\Delta P)_{M_c^{-Ly}} + \mathbb{F}(\Delta P)_{M_c^{+Lz}} + \mathbb{G}(\Delta P)_{M_c^{-Lz}} = \mathbb{S} \tag{III.13}$$

where :

$$\begin{aligned}\mathbb{A} = (J^{1,1})_{M_c^K} &- (J^{1,4})_{M_u^K} \frac{\frac{\partial F^4_{M_u^K}}{\partial P_{M_c^K}}}{\frac{\partial F^4_{M_u^K}}{\partial V^x_{M_u^K}}} - (J^{1,4})_{M_u^{-Lx}} \frac{\frac{\partial F^4_{M_u^{-Lx}}}{\partial P_{M_c^K}}}{\frac{\partial F^4_{M_u^{-Lx}}}{\partial V^x_{M_u^{-Lx}}}} \\ &-(J^{1,5})_{M_v^K} \frac{\frac{\partial F^5_{M_v^K}}{\partial P_{M_c^K}}}{\frac{\partial F^5_{M_v^K}}{\partial V^x_{M_v^K}}} - (J^{1,5})_{M_v^{-Ly}} \frac{\frac{\partial F^5_{M_v^{-Ly}}}{\partial P_{M_c^K}}}{\frac{\partial F^5_{M_v^{-Ly}}}{\partial V^x_{M_v^{-Ly}}}} \\ &-(J^{1,6})_{M_w^K} \frac{\frac{\partial F^6_{M_w^K}}{\partial P_{M_c^K}}}{\frac{\partial F^6_{M_w^K}}{\partial V^x_{M_w^K}}} - (J^{1,6})_{M_w^{-Lz}} \frac{\frac{\partial F^6_{M_w^{-Lz}}}{\partial P_{M_c^K}}}{\frac{\partial F^6_{M_w^{-Lz}}}{\partial V^x_{M_w^{-Lz}}}}\end{aligned}$$

$$\mathbb{B} = -(J^{1,4})_{M_u^K} \frac{\frac{\partial F^4_{M_u^K}}{\partial P_{M_c^{+Lx}}}}{\frac{\partial F^4_{M_u^K}}{\partial V^x_{M_u^K}}} \qquad \mathbb{D} = -(J^{1,5})_{M_v^K} \frac{\frac{\partial F^5_{M_v^K}}{\partial P_{M_c^{+Ly}}}}{\frac{\partial F^5_{M_v^K}}{\partial V^y_{M_v^K}}} \qquad \mathbb{F} = -(J^{1,6})_{M_w^K} \frac{\frac{\partial F^6_{M_w^K}}{\partial P_{M_c^{+Lz}}}}{\frac{\partial F^6_{M_w^K}}{\partial V^z_{M_w^K}}}$$

$$\mathbb{C} = -(J^{1,4})_{M_u^{-Lx}} \frac{\frac{\partial F^4_{M_u^{-Lx}}}{\partial P_{M_c^{-Lx}}}}{\frac{\partial F^4_{M_u^{-Lx}}}{\partial V^x_{M_u^{-Lx}}}} \qquad \mathbb{E} = -(J^{1,5})_{M_v^{-Ly}} \frac{\frac{\partial F^5_{M_v^{-Ly}}}{\partial P_{M_c^{-Ly}}}}{\frac{\partial F^5_{M_v^{-Ly}}}{\partial V^y_{M_v^{-Ly}}}} \qquad \mathbb{G} = -(J^{1,6})_{M_w^{-Lz}} \frac{\frac{\partial F^6_{M_w^{-Lz}}}{\partial P_{M_c^{-Lz}}}}{\frac{\partial F^6_{M_w^{-Lz}}}{\partial V^z_{M_w^{-Lz}}}}$$

$$\mathbb{S} = D^1_{M_c^K} - [\frac{(J^{1,4})_{M_u^K} S^4_{M_u^K}}{\frac{\partial F^4_{M_u^K}}{\partial V^x_{M_u^K}}} + \frac{(J^{1,4})_{M_u^{-Lx}} S^4_{M_u^{-Lx}}}{\frac{\partial F^4_{M_u^{-Lx}}}{\partial V^x_{M_u^{-Lx}}}} + \frac{(J^{1,5})_{M_v^K} S^5_{M_v^K}}{\frac{\partial F^5_{M_v^K}}{\partial V^y_{M_v^K}}} + \frac{(J^{1,5})_{M_v^{-Ly}} S^5_{M_v^{-Ly}}}{\frac{\partial F^5_{M_v^{-Ly}}}{\partial V^y_{M_v^{-Ly}}}}$$
$$+ \frac{(J^{1,6})_{M_w^K} S^6_{M_w^K}}{\frac{\partial F^6_{M_w^K}}{\partial V^z_{M_w^K}}} + \frac{(J^{1,6})_{M_w^{-Lz}} S^6_{M_w^{-Lz}}}{\frac{\partial F^6_{M_w^{-Lz}}}{\partial V^z_{M_w^{-Lz}}}}]$$

As a solution of this equation, the pressure increments will be used to compute the velocity increments thanks to (III.7) and (III.8).

III.3.3 Incréments d'enthalpie et de concentration

To compute the enthalpy increments all we need is to develop the second row of the system (III.11):

$$(J^{3,1})_{M_c^K}(\Delta P)_{M_c^K} + \frac{\partial F^3_{M_c^K}}{\partial h_{M_c^K}}(\Delta h)_{M_c^K} + \frac{\partial F^3_{M_c^K}}{\partial (V^x)_{M_u^K}}(\Delta V^x)_{M_u^K} + \frac{\partial F^3_{M_c^K}}{\partial (V^x)_{M_u^{-Lx}}}(\Delta V^x)_{M_u^{-Lx}}$$
$$+ \frac{\partial F^3_{M_c^K}}{\partial (V^y)_{M_v^K}}(\Delta V^y)_{M_v^K} + \frac{\partial F^3_{M_c^K}}{\partial (V^y)_{M_v^{-Ly}}}(\Delta V^y)_{M_v^{-Ly}} \qquad \text{(III.14)}$$
$$+ \frac{\partial F^3_{M_c^K}}{\partial (V^z)_{M_w^K}}(\Delta V^z)_{M_w^K} + \frac{\partial F^3_{M_c^K}}{\partial (V^z)_{M_w^{-Lz}}}(\Delta V^z)_{M_w^{-Lz}} = D^2_{M_c^K}$$

In the equation (III.14), the pressure increments and the velocity increments are supposed to be known (see sectionIII.3.2). Then only the enthalpy increments are unknown and they can be computed as follows:

$$(\Delta h)_{M_c^K} = \frac{1}{\frac{\partial F^3_{M_c^K}}{\partial h_{M_c^K}}}[D^2_{M_c^K} - \frac{\partial F^3_{M_c^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} - \frac{\partial F^3_{M_c^K}}{\partial (V^x)_{M_u^K}}(\Delta V^x)_{M_u^K} - \frac{\partial F^3_{M_c^K}}{\partial (V^x)_{M_u^{-Lx}}}(\Delta V^x)_{M_u^{-Lx}}$$
$$- \frac{\partial F^3_{M_c^K}}{\partial (V^y)_{M_v^K}}(\Delta V^y)_{M_v^K} - \frac{\partial F^3_{M_c^K}}{\partial (V^y)_{M_v^{-Ly}}}(\Delta V^y)_{M_v^{-Ly}} \qquad \text{(III.15)}$$
$$- \frac{\partial F^3_{M_c^K}}{\partial (V^z)_{M_w^K}}(\Delta V^z)_{M_w^K} - \frac{\partial F^3_{M_c^K}}{\partial (V^z)_{M_w^{-Lz}}}(\Delta V^z)_{M_w^{-Lz}}]$$

The same method applies for the concentration increments that can be computed using the

following relationship:

$$
\begin{aligned}
(\Delta C)_{M_c^K} = \frac{1}{\frac{\partial F^2_{M_c^K}}{\partial C_{M_c^K}}}[D^3_{M_c^K} &- \frac{\partial F^2_{M_c^K}}{\partial P_{M_c^K}}(\Delta P)_{M_c^K} - \frac{\partial F^2_{M_c^K}}{\partial h_{M_c^K}}(\Delta h)_{M_c^K} \\
&- \frac{\partial F^2_{M_c^K}}{\partial (V^x)_{M_u^K}}(\Delta V^x)_{M_u^K} - \frac{\partial F^2_{M_c^K}}{\partial (V^x)_{M_u^{-Lx}}}(\Delta V^x)_{M_u^{-Lx}} \\
&- \frac{\partial F^2_{M_c^K}}{\partial (V^y)_{M_v^K}}(\Delta V^y)_{M_v^K} - \frac{\partial F^2_{M_c^K}}{\partial (V^y)_{M_v^{-Ly}}}(\Delta V^y)_{M_v^{-Ly}} \\
&- \frac{\partial F^2_{M_c^K}}{\partial (V^z)_{M_w^K}}(\Delta V^z)_{M_w^K} - \frac{\partial F^2_{M_c^K}}{\partial (V^z)_{M_w^{-Lz}}}(\Delta V^z)_{M_w^{-Lz}}]
\end{aligned}
\tag{III.16}
$$

III.3.4 Consistency

Before applying the "pressure-based method" it is necessary to ensure its consistency. To do so we consider the simplified moment equation in one dimension :

$$
\frac{V^{n+1}_{M_u^K} - V^n_{M_u^K}}{\Delta t} + \frac{1}{\Delta x}\left[\left((V^D)^{n+1}_{M_c^{+Lx}}(V^M)^{n+1}_{M_c^{+Lx}} - (V^D)^{n+1}_{M_c^K}(V^M)^{n+1}_{M_c^K}\right) + (V)^{n+1}_{M_u^K}\left((V^M)^{n+1}_{M_c^{+Lx}} - (V^M)^{n+1}_{M_c^K}\right)\right] = 0
\tag{III.17}
$$

with:

$$
(V^M)^{n+1}_{M_c^K} = \frac{V^{n+1}_{M_u^K} + V^n_{M_u^{-Lx}}}{2} \quad ; \quad (V^M)^{n+1}_{M_c^{+Lx}} = \frac{V^n_{M_u^{+Lx}} + V^{n+1}_{M_u^K}}{2}
$$

$$
(V^D)^{n+1}_{M_c^K} = \begin{cases} V^n_{M_u^{-Lx}} & if\ (V^M)^{n+1}_{M_c^K} > 0 \\ V^{n+1}_{M_u^K} & otherwise \end{cases}
$$

$$
(V^D)^{n+1}_{M_c^{+Lx}} = \begin{cases} V^{n+1}_{M_u^K} & if\ (V^M)^{n+1}_{M_c^K} > 0 \\ V^n_{M_u^{+Lx}} & otherwise \end{cases}
$$

We assume that $(V^M)^{n+1}_{M_c^K} > 0$ and $(V^M)^{n+1}_{M_c^K}$. The equation III.17 becomes:

$$
\frac{V^{n+1}_{M_u^K} - V^n_{M_u^K}}{\Delta t} + \frac{(V^{n+1}_{M_u^K})^2 - (V^n_{M_u^{-Lx}})^2}{2\Delta x} = 0
\tag{III.18}
$$

$$
\Rightarrow \frac{V^{n+1}_{M_u^K} - V^n_{M_u^K}}{\Delta t} + \frac{(V^{n+1}_{M_u^K})^2 - (V^n_{M_u^K})^2}{2\Delta x} + \frac{(V^n_{M_u^K})^2 - (V^n_{M_u^{-Lx}})^2}{2\Delta x} = 0
$$

$\Rightarrow$ Using a Taylor expansion such that $CFL = \frac{\Delta t|V|}{\Delta x}$ we have :

$$\frac{\partial V}{\partial t}\left(1 + CFL\frac{V}{|V|}\right) + \left[\frac{\partial(V \times V)}{\partial x} - V\frac{\partial V}{\partial x}\right] + \Theta(\Delta x) + \Theta(\Delta t) = 0$$

Then the consistency given by the truncation error $e = \frac{\partial V}{\partial t}\ CFL\ \frac{V}{|V|} + \Theta(\Delta x) + \Theta(\Delta t)$ is obtained when $CFL = 0$.

III.3.5 Key variables

In this step we determine the converged [1] key variables of the porous 4 equations model (I.26):

- the pressure field P using the pressure increments;
- the enthalpy field h using the enthalpy increments;
- the concentration field C using the concentration increments;
- the velocity field $\overrightarrow{V}$ using the velocity increments.

Once the variables P, h, C and $\overrightarrow{V}$ are known, we easily compute the rest of the variables of the model:

- the density field and the internal energy field using the equations of state(I.27);
- the phase variables using the mixture variables.

[1] Convergence if $\Delta\mathcal{U}^{k+1} = \mathcal{U}^{k+1} - \mathcal{U}^{k} < \epsilon$ where ϵ is the user's desired convergence criterion

Chapter IV

Numerical test

To check out the efficiency of the numerical method described in chapters II and III we realize different 1-D tests:

The physical quantities that we use in these tests matches the functioning of the Pressurized Water Reactors or PWR.
We consider a 4.2 m length channel heated by a thermal flux Q constant in time and space and a stiffened gas fluid ([4]) on which we impose the following conditions :

- Zero inlet gas concentration $C_i = 0$
- Constant inlet enthalpies $h_{li} = 1.310^6\ J/kg$ and $h_{vi} = 2.610^6\ J/kg$
- Constant outlet pressure $P_o = 155\ bars$
- Positive inlet velocities $u_{li} > 0$ and $u_{vi} > 0$

The table below gives the details of the realized tests.

Test	Chanel simple	Low inlet velocity	Porosity	Charge loss	Channel complete
$Q\,(W)$	10^8	7.5×10^6	0	0	10^8
$u_i\,(m.s^{-1})$	1	0.01	1	1	1
$g\,(m.s^{-2})$	-9.81	-9.81	0	0	-9.81
ϕ	$[1;1;1]$	$[1;1;1]$	$[1, 0.5, 1]$	$[1;1;1]$	$[1; 0.5; 1]$
K	0	0	0	5	5

To realize each of the tests we make use of the "Full Jacobian" and "pressure-base" methods. We also compare the Ishii and the slip models of the relative velocity. The analytic solutions are given in section see section IV.1

IV.1 Analytic solutions

According to [4], the analytic solutions are given by:

$$h^{\infty}(z) = h_e + \int_0^z Q(y)\, dy \tag{IV.1}$$

$$\rho(h^{\infty}(z), P_0) = \begin{cases} \rho_l(h^{\infty}(z), P_0) & if\ h^{\infty}(z) \leq h_l^s \\ \frac{\rho_l^s \rho_l^s (h_v^s - h_l^s)}{\rho_v^s h_v^s - \rho_l^s h_l^s - h^{\infty}(z)(\rho_v^s - \rho_l^s)} & if\ h_l^s \leq h^{\infty}(z) \leq h_v^s \\ \rho_v(h^{\infty}(z), P_0) & if\ h^{\infty}(z) \geq h_v^s(P_0) \end{cases} \tag{IV.2}$$

$$\alpha(h^{\infty}(z), P_0) = \begin{cases} 0 & if\ h^{\infty}(z) \leq h_l^s \\ \frac{\rho_l^s (h^{\infty}(z) - h_l^s)}{\rho_v^s h_v^s - \rho_l^s h_l^s - h^{\infty}(z)(\rho_v^s - \rho_l^s)} & if\ h_l^s \leq h^{\infty}(z) \leq h_v^s \\ 1 & if\ h^{\infty}(z) \geq h_v^s(P_0) \end{cases} \tag{IV.3}$$

$$u^{\infty}(z) = \frac{D_i}{\rho(h^{\infty}(z), p0)} \qquad such\, that\ D_i = u_i\, \rho(h_i, p0) \tag{IV.4}$$

$$P^{\infty}(z) = P_0 + g \int_z^L \rho(h^{\infty}(y), P_0)\, dy + \left[\frac{(D_i^2)}{\rho(h^{\infty}(y), P_0)} \right]_{y=z}^{y=L} \tag{IV.5}$$

The quantities $h_l^s = h_l^s(P_0)$, $h_v^s = h_v^s(P_0)$, $\rho_l^s = \rho_l^s(P_0)$ and $\rho_v^s = \rho_v^s(P_0)$ are computed using the stiffened gas's state laws(see [4]).

Channel simple

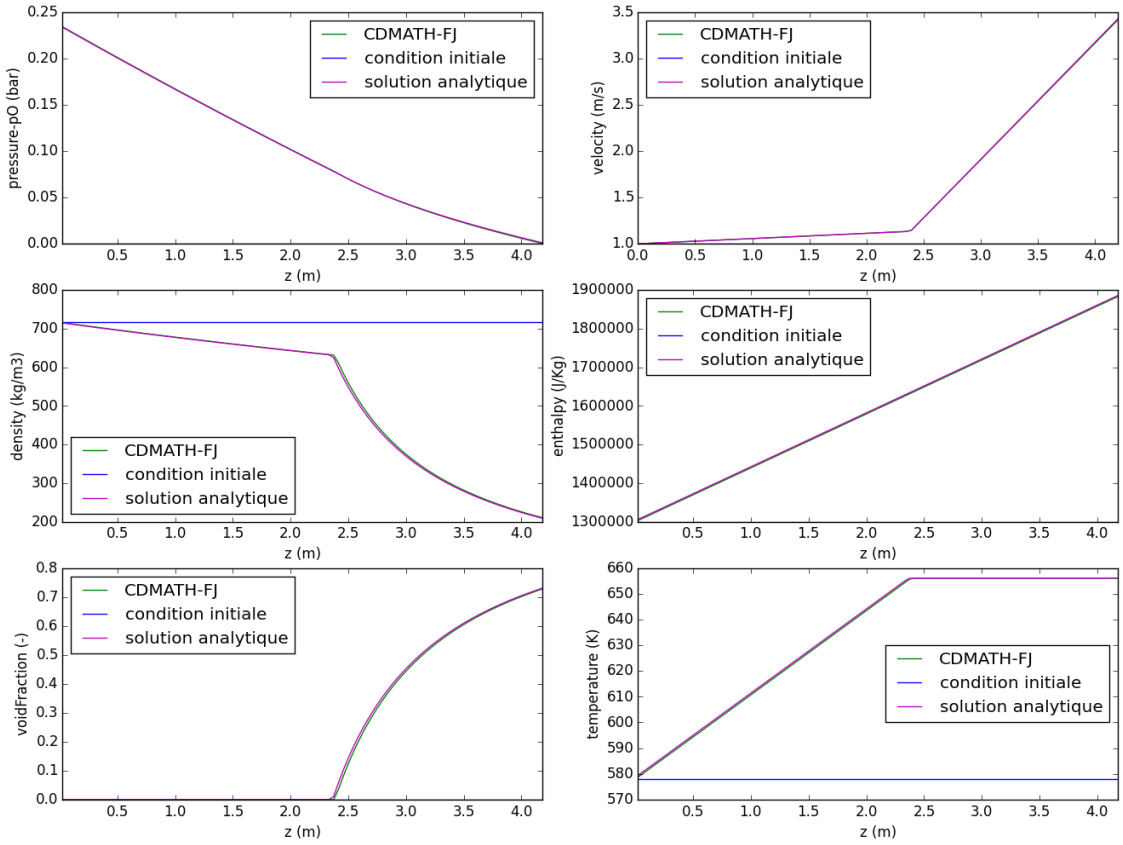

Fig. IV.1 : Channel simple/slip model

Porosity

At the stationary state and according to the mass equation we have:

$$\frac{\partial \rho}{\partial t} = 0 \quad \Rightarrow \quad \frac{\partial \phi \rho V}{\partial x} = 0$$

$$\Rightarrow \phi \rho V = cst$$

Yet ρ varies little in space(then considered as a constant) then we have

$$\phi V = cst$$

$$\Rightarrow V = \frac{cst}{\phi}$$

And since $\phi = [1, 0.5, 1]$ (constant piecewise function) . Then the velocity is also a constant piecwise function(see figure IV.2).
Porosity is divided by 2 in the middle $\phi_{mid} = \frac{\phi}{2}$ then the velocity is multiplied by 2:

$$V_{mid} = \frac{cst}{\phi_{mid}} = 2\frac{cst}{\phi}$$

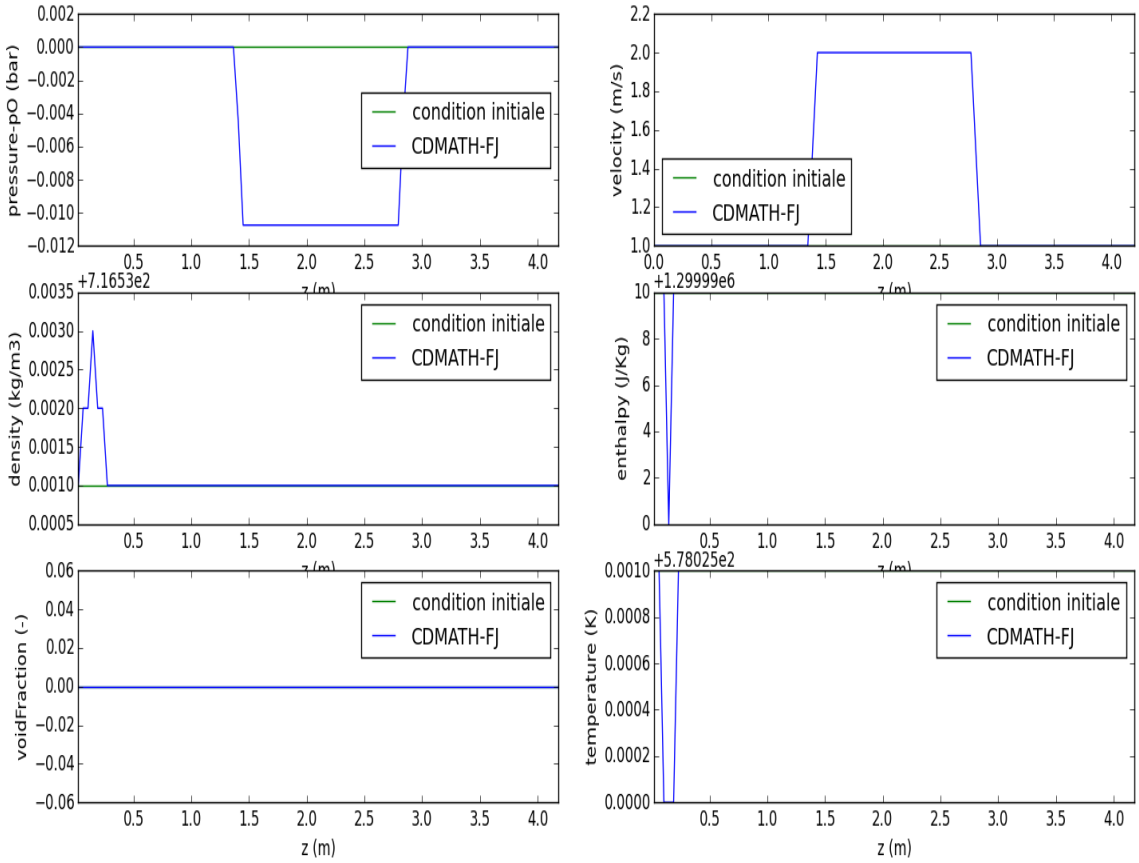

Fig. IV.2 : Porosity/slip model

Charge loss

To compute the pressure drop due to the charge loss we recall the expression of the singular charge loss:

$$\tau_s = \frac{-K}{2\Delta x}\rho V|V|1_{x=x_s}$$

At the stationary state the mass equation implies that the velocity is constant in space. So according to the moment equation we can write:

At $x = x_s$: $\quad \frac{1}{\Delta x}\frac{\partial P}{\partial x} = \tau_s = \frac{-K}{2\Delta x}\rho V|V| \quad \Rightarrow \quad \frac{\partial P}{\partial x} = \frac{-K}{2}\rho V|V|$

$$\Rightarrow P_O - P_{x_s} = \frac{-K}{2}\rho V|V|\Delta x = \frac{-5}{2} \times (0.002 \times 716.53 \times 1 \times 1) \times (4.2/100) \simeq 18.655$$

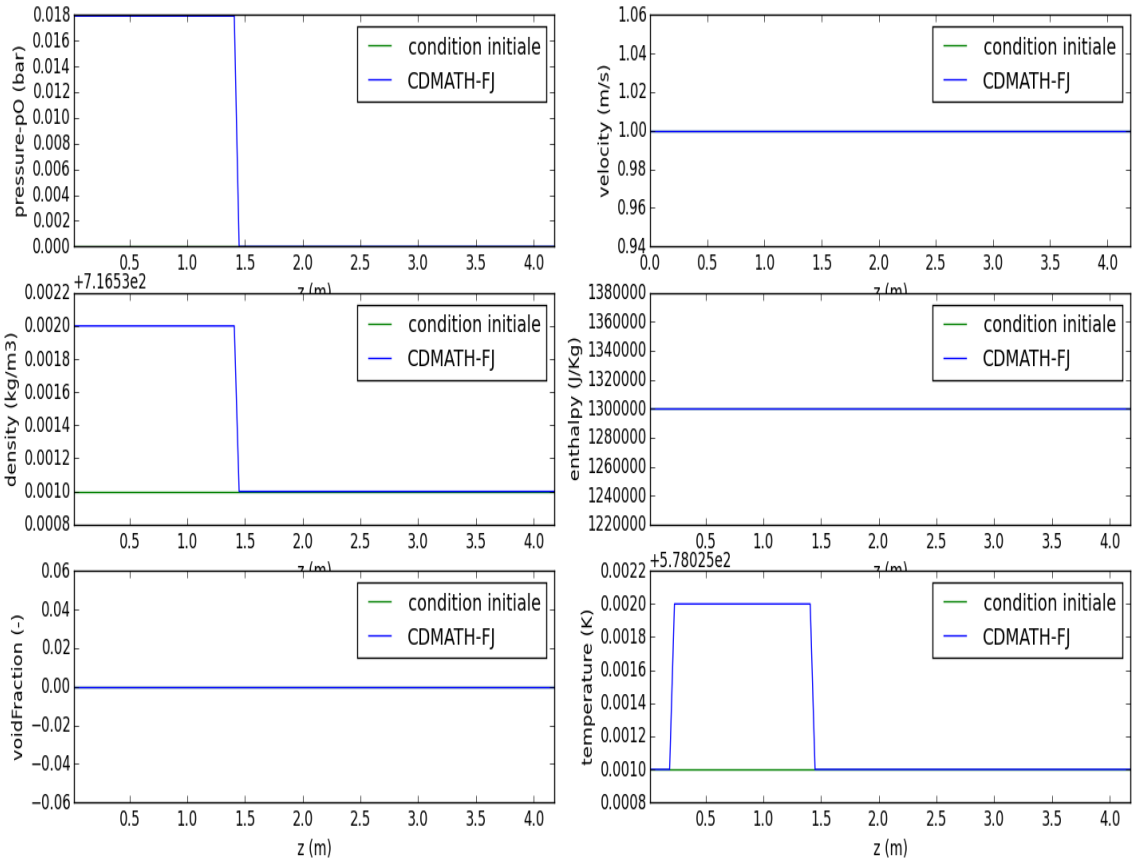

Fig. IV.3 : Charge loss/slip model

Channel complete

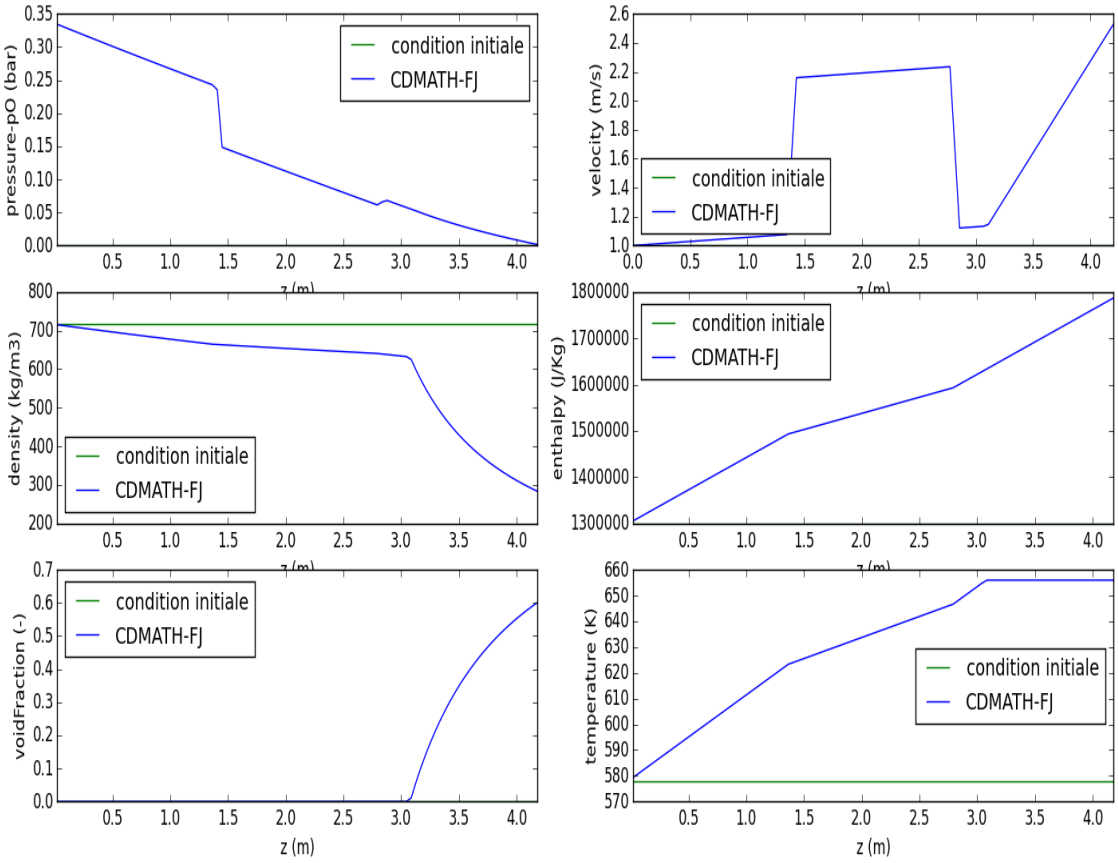

Fig. IV.4 : Channel complete/slip model

Conclusions

In this project we elaborated and implemented the "pressure-based solver" and the "full-jacobian method"(see chapters II and III) based on a staggered grid to solve a two-phase 4 equation model(see chapter I). Different tests have been realized to verify the efficiency of the method in question. The results seem quite promising(see chapter IV).

In my internship I had the chance to discover what working in a reputable research center like CEA looks like. There I was able to put into practice many things that I had learned in class especially the numerical analysis and computing science courses and of course I learned many things that make me love more and more working in the applied mathematics field.

Bibliography

[1] A. Bergeron, Ph. Fillion, D. Gallo, and E. Royer. Flica4 v1.8. modèles physiques. Note Technique SFME/LETR/RT/02-005/A, CEA, 2005.

[2] M. Chandesris. 3d module of cathare : improvement of the momentum convective term discretization. Note Technique DER/SSTH/LDLD/EM/NT/2010-035/A, CEA, 2010.

[3] S. Clerc and Ph. Fillion. Flica4 v1.8. méthode numérique. Note Technique SFME/LETR/RT/02-005/A, CEA, 2001.

[4] Stéphane Dellacherie, Gloria Faccanoni, Bérénice Grec, and Yohan Penel. Study of a low Mach nuclear core model for two-phase flows with phase transition I: stiffened gas law. January 2015.

[5] O. Grégoire. établissement formel d'un modèle diphasique macroscopique à 6 équations, lien avec le modèle macroscopique à 4 équations flica4. Note Technique SFME/LETR/RT/04-007/A, CEA, 2004.