Diagrams finished volumes SUSHI for the modeling of the miscible unsaturated flows

Summary:

This note briefly presents the diagrams finished volumes developed in Code_Aster. A short recall of the equations of behavior concerned is carried out then the diagrams used are presented.

Contents

1 Introduction

We present here the diagrams finished volumes SUSHI developed for the modeling of the diphasic flows (unsaturated) miscible in porous environment, miscible meaning here that the components can exist under several phases. These diagrams concern the family of modelings THM. They are planned only for pure hydraulics (neither mechanics, nor thermics), that is to say if one takes again the classical nomenclature described in [R7.01.11] KIT_HH.

The diagrams finished volumes SUSHI (Design Using Stabilization and Hybrid Interfaces) were developed by Ophélie Angelini within the framework of his thesis [1] in particular to deal with stiff problems of faces on unspecified grids. This diagram is inspired by the diagram Hybid Finite Volume (HVF) introduced by R. Eymard et al.[4]. At the origin of this work, an abundant literature was indicating that these diagrams ensuring by definition a good representation of flow were adapted to this kind of hyperbolic equations applied to strongly heterogeneous fields. To establish and have such diagrams thus quickly appeared reasonable would be to only compare itself with the members of the community of the flows in porous environment [2]. These diagrams do not claim to replace the finite elements but propose a robust alternative.

We will present here only briefly the physical model of the diphasic flows detailed in documentation [R7.01.11].

This documentation thus presents primarily the diagrams of space discretization Finished Volumes implemented on these models in Code_Aster. For further details, one will refer to the thesis of Ophélie Angélini [1]

2 Presentation of the problem: Assumptions, Notations

The whole of the hydraulic physical model is presented in detail in R7.01.11. One is satisfied here to point out the principal variables and assumptions as well as the treated equations. The formalism is primarily resulting from work of Coussy [5]. The routines managing the laws of behavior are not impacted by the use of the diagram finished volume.

2.1 Tally of modeling

These developments relate to only the models with 2 phases (liquid gas) and 2 miscible components (for example water and hydrogen). We thus place ourselves within the framework of modelings *_HH2 (cf U2.04.05). More precisely one will speak here about modeling HH2SUDA (cf section 4).

It is pointed out that the 2 hydraulic laws of behavior that one can use are then:

- LIQU_AD_GAZ_VAPE : 2 components per phase
- LIQU_AD_GAZ : 2 components in the liquid phase, only one in the phase gas (neglected vapor)

In the continuation one will speak only about the complete model with 2 components, 2 phases. The case without vapor amounts right cancelling the terms relating to it.

2.2 Notations

We suppose that the pores of the solid are occupied by two noted components w (for water) and h (for hydrogen), each one coexistent in two phases to the maximum, one liquidate noted l and the other gas one noted g.

Sizes A associated with the phase p ($p=l,g$) component c will be noted: X_p^c. Concretely, that gives:

- A_l^w : size A for liquid water,

- A_g^w : size A for the steam,
- A_l^h : size A for the component H dissolved in the liquid,
- A_g^h : size A for the component H in gas form (e.g. dry hydrogen).

The general assumptions carried out are the following ones:

- anisotropic behavior,
- the gases are perfect gases,
- ideal mixture of perfect gases (total pressure = nap of the partial pressures),
- thermodynamic balance between the phases of the same component.

The various notations are clarified hereafter.

2.2.1.1 Variables of state

The variables are:

- pressures of each components P_p^c
- the temperature of the medium T.

These various variables are not completely independent. Indeed, if only one component is considered, thermodynamic balance between its phases imposes a relation between the steam pressure and the pressure of the liquid of this component. Finally, there is only one independent pressure per component, just as there is only one conservation equation of the mass. The number of independent pressures is thus equal to the number of independent components. The choice of these pressures is free (combinations of the pressures of the components) provided that the pressures chosen, associated with the temperature, form a system of independent variables.

We chose - and in order to be homogeneous with the finite elements formulation - as variable independent and descriptive of the medium:

- total pressure of gas $P_g = P_g^w + P_g^h$, (law of Dalton)
- Total pressure of liquid $P_l = P_l^w + P_l^h$
- capillary pressure $P_c = P_g - P_l = P_g^w + P_g^h - (P_l^w + P_l^h)$.

2.2.1.2 Sizes characteristic of the solid phase

One notes:

Porosity: ϕ ,

The intrinsic tensor of permeability: $\boldsymbol{k}$

2.2.1.3 Sizes characteristic of the fluids

One notes:

- Density of the phase p : ρ_p , $\rho_p = \rho_p^w + \rho_p^h$
- The viscosity of the phase p : μ_p
- The saturation of the phase p : , $S_l + S_g = 1$ who is a decreasing function of the capillary pressure. One thus has $S_l = f\left(P_c\right)$.
- The relative permeability of the phase p : k_{rp} function of saturation

- The hydraulic conductivity of the phase p : λ_p^H such as: $\lambda_p^H=\frac{\boldsymbol{k}\,k_{rp}}{\mu_p}$
- The mobility of the component $c, c=(h,w)$ associated with the phase p $k_p^c=\frac{\rho_p^c k_{rp}}{\mu_p}$
- Molar mass of the component c : M^c
- Molar concentration $c_p^c=\frac{\rho_p^c}{M^c}$
- Mass fraction of the phase p and of the component c : $\zeta_p^c=\frac{\rho_p^c}{\rho_p}$
- Molar fraction: $X_p^c=\frac{c_p^c}{c_p}$ where $c_p=c_p^h+c_p^w$ (in the literature, these concentrations are sometimes also noted C_p^c)
- The module of compressibility of water K_w

2.3 Equations constitutive of the model

One will not give the details here allowing to arrive at the final equations of the model. For the intermediate stages, one will refer to [R7.01.11]. One is thus satisfied here with a brief recall with principal equations.

2.3.1 Equilibrium equations

The equilibrium equations are given here by the conservation of the mass of each component, is:

$$\begin{cases} \dot{m}_l^w+\dot{m}_g^w+Div\left(\boldsymbol{F}_l^w+\boldsymbol{F}_g^w\right)=0 \\ \dot{m}_l^h+\dot{m}_g^h+Div\left(\boldsymbol{F}_l^h+\boldsymbol{F}_g^h\right)=0 \end{cases}$$

with m_p^c the mass contribution of the component c in phase p , such as $m_p^c=\phi.S_p.\rho_p^c$ and $\boldsymbol{F}_p^c$ the mass flow of the phase p for the component c .

$\boldsymbol{F}_p^c$ is made up by mass flow Fickien $\boldsymbol{J}_p^c$ and of mass flow Darcéen $\boldsymbol{F}_p$ such as:

$$\boldsymbol{F}_p^c=\boldsymbol{J}_p^c+\rho_p^c\frac{\boldsymbol{F}_p}{\rho_l}, c=(h,w); p=(l,g)$$

2.3.2 Equations of behavior

2.3.2.1 Laws of behavior of the fluids

Evolution of porosity:

In the absence of mechanics, one allows nevertheless an evolution of porosity via the coefficient of storage E_m , such as:

$$d\,\phi=E_m d\,P_l$$

Behavior of the liquid:

It is considered that water can be compressible: $\frac{d\,\rho_l^w}{\rho_l^w}=\frac{dP_l^w}{K_w}$

Gas reaction of:

It is considered that the gas is subjected to the law of perfect gases:

$\frac{P_g^c}{\rho_g^c}=\frac{RT}{M^c};c=(w,h)$ where R is the constant of perfect gases.

Law of balance water vapor:

balance water vapor is written by equality of the free enthali, which, for an isothermal problem gives (confer R7.01.11) :

$$\frac{d\,P_g^w}{\rho_g^w}=\frac{dP_l^w}{\rho_l^w}$$

Law of balance dry gas /dissous:

The law of Henry connects the component c in its gas form with its liquid form such as:

$P_g^h=K_h\frac{\rho_l^h}{M^h}$ where K_h coefficient of Henry.

Note: one often finds this coefficient in the literature in the form $H=\frac{1}{K_h}$

2.3.2.2 Equations of diffusion

Law of Darcy:

The law of Darcy connects flow $\boldsymbol{F_p}$ phase p with its gradient of pressure, such as:

$$\frac{\boldsymbol{F_p}}{\rho_p}=\frac{-\boldsymbol{k}\,k_{rp}}{\mu_p}\left(\nabla P_p-\rho_p\boldsymbol{g}\right)$$

with $\boldsymbol{g}$ gravity

Law of Fick:

One writes mass flows Fickiens such as:

$\boldsymbol{J_p^c}=-\phi M^c S_p D_p c_p \nabla X_p^c$ where D_p is the coefficient of diffusion (where coefficient of Fick) of the phase p .

One neglects Fickien flow of water in the liquid (concentration of water in the liquid comparable to 1). With final, one thus obtains:

$$\boldsymbol{F_l^w}=-\rho_l^w\lambda_l^H\left(\nabla P_l-\rho_l\boldsymbol{g}\right)$$
$$\boldsymbol{F_l^h}=-\rho_l^h\lambda_l^H\left(\nabla P_l-\rho_l\boldsymbol{g}\right)-\phi M^h S_l c_l D_l\nabla X_l^h$$
$$\boldsymbol{F_g^w}=-\rho_g^w\lambda_g^H\left(\nabla P_g-\rho_g\boldsymbol{g}\right)-\phi M^w S_g c_g D_g\nabla X_g^w$$
$$\boldsymbol{F_g^h}=-\rho_g^h\lambda_g^H\left(\nabla P_g-\rho_g\boldsymbol{g}\right)-\phi M^h S_g c_g D_g\nabla X_g^h$$

3 The diagrams finished volumes implemented in *Code_Aster*

We present in this chapter the diagrams finished volumes which were implemented in Code_Aster.

3.1 General information on finished volumes

The method of finished volumes consists in integrating one or more equations on a volume of control then to discretize flows on each edge of these volumes. Contrary to the finite elements, there is not properly spoke about variational formula.
Let us take the example of an equation of the form $div(\Theta(X,u,\nabla u))=f(x)$. Its approximation on a unit $\Omega\subset\mathbb{R}^n$ is a constant function per pieces on a cutting of Ω in volumes of controls noted thereafter K .
The principle of the method of finished volumes is to integrate the equation on each one of these volumes of control. By using the formula of Green, the equations are written:

$$\int_{\partial K}\Theta(X,u,\nabla u).n_K d\gamma=\int_K f(x)dx,\forall K$$

with n_K the outgoing unit normal of the volume of control K .

It is seen whereas to apply a diagram finished volumes consists in approaching flows on edges.
For a transitory equation of the type:
$\frac{\partial u}{\partial t}+div(\Theta(X,u,\nabla u))=f(x)$, there will be logically a formulation of the type
$\int_K u\,dx+\int_{\partial K}\Theta(X,u,\nabla u).n_K d\gamma=\int_K f(x)dx,\forall K$

In short, a diagram finished volumes is defined by:

- The choice of the volume of control K who can be identical to the mesh, or a construction (of Voronoï type for example). The approximate solution given by the diagrams of finished the volumes type will be constant per pieces on this cutting.
- The position of the nodes of approximation of the unknown factors for each volume.
- Manner of approaching flow on an edge of the volume of control: They are approached by the integral formulation of the equations and the application of the formula of Green on the edge of the volume of control. During the approximation, flows must be conservative and consistent. The conservativity results in the continuity of flows to the interface, by definition ensured by finished volumes (flow is written explicitly). Consistency is reached when the difference between real flow and its approximation tends towards 0. There exists one very a large number of diagrams according to the way of calculating this flow and necessary consistency.

The writing of flow can thus to connect nodes which do not belong forcing to the same element. They can be connected for example by a common interface. One thus sees that in this case, two nodes are connected, either when they belong to the same element as in finite elements, but when they belong to two neighbors (connected by a common face).

To implement most these diagrams it is thus necessary to resort to the topological concept of vicinity what constitutes an important difference compared to the finite elements.

3.2 Finished volumes SUSHI applied to the miscible diphasic flows

The diphasic flows in porous environment are governed by the system of equations (3.2.1) :

$$\begin{cases} \dot{m}_l^w + \dot{m}_g^w + Div\left(\boldsymbol{F_l^w} + \boldsymbol{F_g^w}\right) = 0 \\ \dot{m}_l^h + \dot{m}_g^h + Div\left(\boldsymbol{F_l^h} + \boldsymbol{F_g^h}\right) = 0 \\ P_l(\boldsymbol{x}, t) = \tilde{P}_l \quad sur \quad \partial\Omega_d \\ S_l(\boldsymbol{x}, t) = \tilde{S}_l \quad sur \quad \partial\Omega_d \\ [\boldsymbol{F_l^w} + \boldsymbol{F_g^w}].\boldsymbol{n} = \phi^w \quad sur \quad \partial\Omega_n \\ [\boldsymbol{F_l^h} + \boldsymbol{F_g^h}].\boldsymbol{n} = \phi^h \quad sur \quad \partial\Omega_n \end{cases} \tag{3.2.1}$$

It is pointed out in addition that the expression of the mass contributions is:

$$\begin{aligned} m_w &= \rho_w \varphi S_{lq} - \rho_w^0 \varphi^0 S_{lq}^0 \\ m_{ad} &= \rho_{ad} \varphi S_{lq} - \rho_{ad}^0 \varphi^0 S_{lq}^0 \\ m_{as} &= \rho_{as} \varphi\left(1 - S_{lq}\right) - \rho_{as}^0 \varphi^0 \left(1 - S_{lq}^0\right) \\ m_{vp} &= \rho_{vp} \varphi\left(1 - S_{lq}\right) - \rho_{vp}^0 \varphi^0 \left(1 - S_{lq}^0\right) \end{aligned} \tag{3.2.2}$$

flows are then:

$$\begin{aligned} \boldsymbol{F_l^w} &= -\rho_l^w \lambda_l^H \left(\nabla P_l - \rho_l \boldsymbol{g}\right) \\ \boldsymbol{F_l^h} &= -\rho_l^h \lambda_l^H \left(\nabla P_l - \rho_l \boldsymbol{g}\right) - \phi M^h S_l c_l D_l \nabla X_l^h \\ \boldsymbol{F_g^w} &= -\rho_g^w \lambda_g^H \left(\nabla P_g - \rho_g \boldsymbol{g}\right) - \phi M^w S_g c_g D_g \nabla X_g^w \\ \boldsymbol{F_g^h} &= -\rho_g^h \lambda_g^H \left(\nabla P_g - \rho_g \boldsymbol{g}\right) - \phi M^h S_g c_g D_g \nabla X_g^h \end{aligned} \tag{3.2.3}$$

3.2.1 Choice of the unknown factors

The usual choice of unknown factors (P_c, P_g) is retained in the mesh like on the edges of this one. This choice is in addition compatible with the treatment unified miscible and immiscible flows in medium saturated and unsaturated (see [1]).

3.2.2 Choice of the volume of control

The volume of control corresponds here to the grid: an element is equal to a volume of control.

3.2.3 Writing of flows

Geometrical notations used thereafter for an element K (here triangular, but the principle is the same one for rectangle or in 3D) are indicated Illustration 1.
One will note thereafter L the close triangle with K separated by the interface σ. It is pointed out that the notation $|K|$ indicate its measurement (or surfaces).

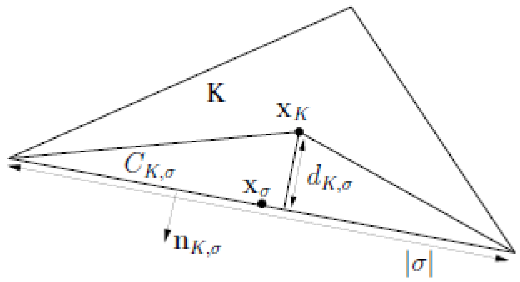

Illustration 1: Representation of the various quantities

We can distinguish various types of flow which we will name thereafter "mass" flows or "voluminal" flows. Mass flows are actually "physical" flows classics in other words they are the quantities $\int_{\partial K} -\boldsymbol{k} k_p^c \nabla [P_p - \rho_p \boldsymbol{g.x}].\boldsymbol{n}_{\boldsymbol{K},\sigma} d\gamma$ for the Darcéens terms and $\int_{\partial K} -\phi M^c S_p D_p(S_p) c_p \nabla X_p^c.\boldsymbol{n}_{\boldsymbol{K},\sigma} d\gamma$ for the Fickiens terms.
On the other hand, voluminal flows are for the Darcéens terms the quantities $\int_{\partial K} -\boldsymbol{k} \nabla [P_p - \rho_p \boldsymbol{g.x}], \boldsymbol{n}_{\boldsymbol{K},\sigma} d\gamma$ and for the Fickiens terms quantities $\int_{\partial K} -\nabla X_p^c.\boldsymbol{n}_{\boldsymbol{K},\sigma} d\gamma$.
Concretely, one extracts the terms depending on space (via saturation) from calculation on voluminal flow.

One of the choices carried out for the extension of the diagram SUSHI to the diphasic nonlinear case is to rather approximate by discrete flows voluminal flows than mass flows. This choice has the advantage of being able to lead to an equation of continuity of linear voluminal flows. However, it is then necessary to ensure the continuity of the other discontinuous quantities step of other techniques (for example, by decentring or average). These various approaches are compared in [1].

One then notes the discretization of voluminal flow such as:

- $\int_{\partial K} -\boldsymbol{k} \nabla [P_p - \rho_p \boldsymbol{g.x}], \boldsymbol{n}_{\boldsymbol{K},\sigma} d\gamma$ is discretized by $\Sigma_{\sigma \in \epsilon_K} F_{p,K,\sigma}(P_p - \rho_p \boldsymbol{g.x}), p \in (l,g)$
  (one summons flows for each edge σ belonging to the whole of stop K: ϵ_K).
- $\int_{\partial K} -\nabla X_p^c.\boldsymbol{n}_{\boldsymbol{K},\sigma} d\gamma$ is discretized by $\Sigma_{\sigma \in \epsilon_K} \tilde{F}_{p,K,\sigma}(X_p^c), c \in (h,w), p \in (l,g)$.

Discretized voluminal flows are thus expressed in the following way:

$$F_{p,K,\sigma}(P_p - \rho_g \boldsymbol{g.x}) = \Sigma_{\sigma' \in \epsilon_K} C_K^{\sigma,\sigma'}[P_{p,K} - P_{p,\sigma'} - \rho_{p,K} \boldsymbol{g}.[\boldsymbol{x_K} - \boldsymbol{x}_{\sigma'}]] \quad (3.2.4)$$

$$\tilde{F}_{p,K,\sigma}(X_p^c) = \sum_{\sigma' \in \epsilon_K} D_K^{\sigma,\sigma'}[X_{p,K}^c - X_{p,\sigma'}^c] \quad (3.2.5)$$

With

$$C_K^{\sigma,\sigma'} = \sum_{\sigma'' \in \epsilon_K} \boldsymbol{Y}^{\sigma'',\sigma}.\boldsymbol{k}_{\boldsymbol{K},\sigma''} \boldsymbol{Y}^{\sigma'',\sigma'} \quad (3.2.6)$$

$$D_K^{\sigma,\sigma'} = \sum_{\sigma'' \in \epsilon_K} \boldsymbol{Y}^{\sigma'',\sigma}.\frac{d_{K,\sigma''}|\sigma''|}{d} \boldsymbol{Y}^{\sigma'',\sigma'} \quad (3.2.7)$$

Where:

$$\boldsymbol{k}_{\boldsymbol{K},\sigma''} = \int_{C_{K,\sigma}} \boldsymbol{k}(\boldsymbol{x}) d\,\boldsymbol{x} = \boldsymbol{k}_{\boldsymbol{K}} \frac{d_{K,\sigma''}|\sigma''|}{d} \quad (3.2.8)$$

And:

$$\boldsymbol{Y}^{\sigma,\sigma'}=\frac{|\sigma|}{|K|}\boldsymbol{n}_{K,\sigma}+\frac{\beta_K}{d_{k,\sigma}}[1-\frac{|\sigma|}{|K|}\boldsymbol{n}_{K,\sigma}.[\boldsymbol{x}_\sigma-\boldsymbol{x}_K]]\boldsymbol{n}_{k,\sigma} \quad si \quad \sigma=\sigma' \qquad (3.2.9)$$

$$\boldsymbol{Y}^{\sigma,\sigma'}=\frac{|\sigma'|}{|K|}\boldsymbol{n}_{K,\sigma'}-\frac{\beta_K}{d_{k,\sigma}|K|}|\sigma'|\boldsymbol{n}_{K,\sigma'}.[\boldsymbol{x}_\sigma-\boldsymbol{x}_K]\boldsymbol{n}_{k,\sigma} \quad si \quad \sigma\neq\sigma' \qquad (3.2.10)$$

The choice to discretize by the method of Finished Volumes SUSHI only voluminal flows results in having to treat in a specific way mobilities as well as the terms of Fickiens diffusion. Indeed, the relative permeabilities as well as the tensors of diffusion, present respectively in mobilities and the terms of Fickiens diffusion, are quantities which depend on saturation and which can be heterogeneous.

We will present various possible formulations of the discretization of the equations which govern the flows in porous environment, resulting from various decentrings of the nonlinear quantities.

One will note thereafter:

- The equation discretized of conservation of water on the element K : R_K^w
- The equation discretized of conservation of the component gas on the element K : R_K^h
- The equation discretized of continuity of the water flow through the interface σ : R_σ^w
- The equation discretized of continuity of the flow of the gas component through the interface σ : R_σ^h

3.2.4 Decentring

The phenomenon dominating in the diphasic flows in porous environment is the diffusion Darcéenne, we will thus focus itself on the study of the continuity of mobilities $\rho_p\frac{k_{r,p}}{\mu_p}$. The terms of Fickiens diffusion will be looked in the second place so only ensuring their assured continuity once that of mobilities.

When we are in the presence of nonlinear terms which depend on space, here mobilities, we must ensure their continuity in the event of heterogeneous problem. For that we can decentre them. The decentring of mobilities aims to ensure the monotony and the stability of the diagrams. However, it decreases the precision of calculations by adding digital diffusion. There exist many decentrings in the literature, the nonlinear term of mobility $\rho_p\frac{k_{r,p}}{\mu_p}$ depending on space, being able to be calculated by various diagrams:

- the diagram upstream which decentres this term according to the direction of the flow of the phase in the current mesh or the close mesh by the edge considered,
- the causal diagram which will decentre this term differently when it is factor of a term of pressure or factor of a term of gravity. Decentring will be done all the same in the current mesh or the close mesh,
- the diagram with Peclet number variable who allows to break up the convective part of flow into a linear combination between the eccentric flow of the diagram upstream and centered flow. Thus the parameter of this combination can be adjusted locally on each edge according to the diffusion introduced by the capillary pressure.

We will present the formulations below retained in Code_Aster.
Initially 3 formulations were implemented in Code_Aster: two of them will decentre by the diagram upstream mobilities, either on the edge of the current mesh or on the close mesh by the edge and the third formulation will use the mobilities centered in the current mesh.
We decided to preserve a single formulation (for reason of stability and computing time): the formulation eccentric edge.

Formulation: diagram Volumes Finis Décentré Arête (VFDA)

The interest of this formulation is at the same time to keep the concept of decentring, while keeping a small stencil of the matrix jacobienne. For that, we continue to write the continuity of mass total flows but we decentre mobilities on the edges of the current mesh. We thus consider the continuity of the following quantities:

$$\int_{\partial K}\left[-\boldsymbol{k}\,k_l^w\nabla[P_l-\rho_l\,\boldsymbol{g}.\boldsymbol{x}]-\boldsymbol{k}\,k_g^w\nabla[P_g-\rho_g\,\boldsymbol{g}.\boldsymbol{x}]-\phi M^w S_g D_g c_g\nabla X_g^w\right].\boldsymbol{n}_{\boldsymbol{K},\sigma}\,d\gamma$$

and

$$\int_{\partial K}\left[-\boldsymbol{k}\,k_l^h\nabla[P_l-\rho_l\,\boldsymbol{g}.\boldsymbol{x}]-\boldsymbol{k}\,k_g^h\nabla[P_g-\rho_g\,\boldsymbol{g}.\boldsymbol{x}]-\phi M^h S_g D_g c_g\nabla X_g^h-\phi M^h S_l D_l c_l\nabla X_l^h\right].\boldsymbol{n}_{\boldsymbol{K},\sigma}\,d\gamma$$

Decentring is written then:

$$\begin{array}{l} Si \quad F_{p,K,\sigma}\geqslant 0 \quad alors \quad k_{p,K,\sigma}^c=k_p^c(P_{p,K}) \\ Si \quad F_{p,K,\sigma}<0 \quad alors \quad k_{p,K,\sigma}^c=k_p^c(P_{p,\sigma}) \end{array} \tag{3.2.11}$$

With regard to the terms of Fickiens diffusion, since the molecular diffusion is not the phenomenon dominating, we decide not to apply particular treatment to them and we will thus take their values in the current mesh.

Thus we will be able, in this formulation, not to make the distinction enters the internal edges and the edges of edges. A flat with this formulation could be that final we ensure doubly the continuity of mass flows Darcéens since they are continuous thanks to the equations of continuity of flows but also thanks to their writing in the conservation of the mass.

In spite of that this formulation seems to be able to be powerful. Indeed, it does not use the neighbors of the edges, which enables him to have a weak time of resolution. In addition, it makes it possible to solve heterogeneous problems.

Discretization of the first two equations of the system (3.2.1)is written in the following way:

$$
\left|
\begin{array}{l}
eq.\ R_K^w:\\
\frac{|K|}{\Delta t}[m_{l,K}^w-m_{l,K}^{w,-}]+\frac{|K|}{\Delta t}[m_{g,K}^w-m_{g,K}^{w,-}]+\sum_{\sigma\in\epsilon_{K,ext}}[k_{l,K,\sigma}^w F_{l,K,\sigma}(P_l-\rho_l\boldsymbol{g}.\boldsymbol{x})]\\
+\sum_{\sigma\in\epsilon_{K,ext}}[k_{g,K,\sigma}^w F_{g,K,\sigma}(P_g-\rho_g\boldsymbol{g}.\boldsymbol{x})+\phi_K M^w S_{g,K}D_{g,K,\sigma}c_{g,K}\tilde{F}_{g,K,\sigma}(X_g^w)]=0\\
eq.\ R_\sigma^w:\\
k_{l,K,\sigma}^w F_{l,K,\sigma}(P_l-\rho_l\boldsymbol{g}.\boldsymbol{x})+k_{g,K,\sigma}^w F_{g,K,\sigma}(P_g-\rho_g\boldsymbol{g}.\boldsymbol{x})\\
+\phi_K M^w S_{g,K}D_{g,K,\sigma}c_{g,K}\tilde{F}_{g,K,\sigma}(X_g^w)+k_{l,L,\sigma}^w F_{l,L,\sigma}(P_l-\rho_l\boldsymbol{g}.\boldsymbol{x})\\
+k_{g,L,\sigma}^w F_{g,L,\sigma}(P_g-\rho_g\boldsymbol{g}.\boldsymbol{x})+\phi_L M^w S_{g,L}D_{g,L,\sigma}c_{g,L}\tilde{F}_{g,L,\sigma}(X_g^w)=0\\
\\
eq.\ R_K^h:\\
\frac{|K|}{\Delta t}[m_{l,K}^h-m_{l,K}^{h,-}]+\frac{|K|}{\Delta t}[m_{g,K}^h-m_{g,K}^{h,-}]+\sum_{\sigma\in\epsilon_{K,inter}}[k_{l,K,\sigma}^h F_{l,K,\sigma}(P_l-\rho_l\boldsymbol{g}.\boldsymbol{x})]\\
+\sum_{\sigma\in\epsilon_{K,inter}}[k_{g,K,\sigma}^h F_{g,K,\sigma}(P_g-\rho_g\boldsymbol{g}.\boldsymbol{x})]+\sum_{p\in(l,g)}\phi_K M^h S_{p,K}D_{p,K,\sigma}c_{p,K}\tilde{F}_{p,K,\sigma}(X_p^h)\\
=0\\
eq.\ R_\sigma^h:\\
k_{l,K,\sigma}^h F_{l,K,\sigma}(P_l-\rho_l\boldsymbol{g}.\boldsymbol{x})+k_{g,K,\sigma}^h F_{g,K,\sigma}(P_g-\rho_g\boldsymbol{g}.\boldsymbol{x})\\
+\phi_K M^h S_{g,K}D_{g,K,\sigma}c_{g,K}\tilde{F}_{g,K,\sigma}(X_g^w)+\phi_K M^h S_{l,K}D_{l,K,\sigma}c_{l,K}\tilde{F}_{l,K,\sigma}(X_l^w)\\
k_{l,L,\sigma}^h F_{l,L,\sigma}(P_l-\rho_l\boldsymbol{g}.\boldsymbol{x})+k_{g,L,\sigma}^h F_{g,L,\sigma}(P_g-\rho_g\boldsymbol{g}.\boldsymbol{x})\\
+\phi_L M^h S_{g,L}D_{g,L,\sigma}c_{g,L}\tilde{F}_{g,L,\sigma}(X_g^w)+\phi_L M^h S_{l,L}D_{l,L,\sigma}c_{l,L}\tilde{F}_{l,L,\sigma}(X_l^w)=0
\end{array}
\right.
\quad (3.2.12)
$$

4 Implementation in Code_Aster

In this chapter, we specify how are integrated the relations described into chapter 3.

With**ttention finished volumes are not currently found that with the hydraulic mixing rate `HYDR_VGM` who allows to correctly manage the appearance/disparation of phase by treating negative capillary pressures. Only model hydraulics now available are thus of the type Mualem Van-Genuchten.**

4.1 Description of the elements

2 types of modelings exist according to the diagram used:

Modeling	Corresponding diagram	Compatible law of flow
D_PLAN_HH2SUDA	VFDA	LIQU_AD_GAZ_VAPE, LIQU_AD_GAZ
3D_HH2SUDA	VFDA	LIQU_AD_GAZ_VAPE, LIQU_AD_GAZ

Table 4.1-1: Model finished volumes

The principal unknown factors are the capillary pressure (PRE1) and gas pressure (PRE2) and are located at the center of the meshs like at the mediums of the edges (cf. Illustration 2).

Illustration 2: Quadratic element

What thus gives for a quadrangle a storage of the kind:

Support	DDL
Face $\sigma 1$	PRE1
	PRE2
Face $\sigma 2$	PRE1
	PRE2
Face $\sigma 3$	PRE1
	PRE2
Face $\sigma 4$	PRE1
	PRE2
Center K	PRE1
	PRE2

Table 4.1-2: Storage of the unknown factors

The elements meshs are defined in 2D for triangles with 7 nodes and quadrilaterals with 9 nodes (“unutilised” tops + mediums of stop + center) like in 3D for hexahedrons with 27 nodes.
One does not have elements of grids which would exclude the nodes tops but the latter are not taken into account (cf. Illustration 2).

4.2 Calculation of the constraints and generalized deformations

The diagrams finished volumes profit largely from the definite structure for the finite elements in [R7.01.10] and [R7.01.11].

Thus the constraints generalized in the center of the element are physically the same ones as in finite elements, namely:
$m_l^w, \mathbf{F_l^w}; m_g^w, \mathbf{F_g^w}; m_g^h, \mathbf{F_g^h}; m_l^h, \mathbf{F_l^h}$ as well as the generalized deformations: $p_c, \nabla p_c; p_g, \nabla p_g$.

With the interfaces on the other hand, flows contain in fact the necessary one to the equation of continuity. This last can be different according to the diagram used (see section 3.2.4).

Name of component Aster	Contents in the center of K	Contents on the faces $\sigma\in\delta K$
M11	$\rho_l^w \varphi S_l-(\rho_l^w \varphi S_l)^-$	0
FH11*	$\sum_{\delta K} \boldsymbol{F}_l^w.\boldsymbol{n}$	$\boldsymbol{F}_l^w.\boldsymbol{n}_{K,\sigma}+\boldsymbol{F}_g^w.\boldsymbol{n}_{K,\sigma}$
M12	$\rho_g^w \varphi S_g-(\rho_g^w \varphi S_g)^-$	0
FH12*	$\sum_{\delta K} \boldsymbol{F}_g^w.\boldsymbol{n}$	$\boldsymbol{F}_l^h.\boldsymbol{n}_{K,\sigma}+\boldsymbol{F}_g^h.\boldsymbol{n}_{K,\sigma}$
M21	$\rho_g^h \varphi S_l-(\rho_g^h \varphi S_g)^-$	0
FH21*	$\sum_{\delta K} \boldsymbol{F}_g^h.\boldsymbol{n}$	0
M22	$\rho_l^h \varphi S_l-(\rho_l^h \varphi S_l)^-$	0
FH22*	$\sum_{\delta K} \boldsymbol{F}_l^h.\boldsymbol{n}$	0

Table 4.2-1: Constraints generalized for diagrams VFDA (*`HH2SUDA`)

4.3 Integration

As in finite elements, the principal loop of integration is done by element. On the other hand within an element one will buckle on the nodes (there is no more concept of points of integration, but just of the points of approximation which are the nodes here). This diagram having its nodes in the center like on each edge, that makes it possible here implicitly to make a loop on the interfaces. Finally, the structure finite elements is not modified.

With final one can summarize the integration of the various equations treated in the following table (written for a quadrangle but easily generalizable):

Support	Equation	Type
Face $\sigma 1$	$R_{\sigma 1}^w$	Continuity flow of water
	$R_{\sigma 1}^h$	Continuity flow of h
Face $\sigma 2$	$R_{\sigma 2}^w$	Continuity flow of water
	$R_{\sigma 2}^h$	Continuity flow of h
Face $\sigma 3$	$R_{\sigma 3}^w$	Continuity flow of water
	$R_{\sigma 3}^h$	Continuity flow of h
Face $\sigma 4$	$R_{\sigma 4}^w$	Continuity flow of water
	$R_{\sigma 4}^h$	Continuity flow of h
Center K	R_K^w	Conservation of the mass of water

	R_K^h	Conservation of the mass of h

4.4 Internal variables

The internal variables are here:

Number	Name of component Aster	Contents
1	$V1$	$\rho_{lq}-\rho_{lq}^0$
2	$V2$	$\varphi-\varphi^0$
3	$V3$	$p_{vp}-p_{vp}^0$
4	$V4$	S_{lq}
5	$V5$	P_c
6	$V6$	P_g

Notice : it is pointed out that here the points of Gauss to the direction Aster are the nodes of the element.

4.5 Validation

The following table presents some examples of case tests of validation for classical physical problems:

Case test	Phenomenon	Modelings tested
wtnp117	Capillary rebalancing	D_PLAN_HH2SUDA (c)
wtnp120	Appearance/disappearance of phase in a bar	D_PLAN_HH2SUDA (A) 3D_HH2SUDA (c)
wtnp121	Bar saturated with water subjected to a shock with pressure	D_PLAN_HH2SUDA (A) 3D_HH2SUDA (E)
wtnp122	Bar saturated with gas subjected to a shock with pressure	D_PLAN_HH2SUDA (A)
wtnp123	Gas goshawks injection of a gallery	D_PLAN_HH2SUDA (A)
wtnp124	Test of Liakopoulos: gravitating drainage of a water column	D_PLAN_HH2SUDA (A)

5 Bibliography

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6 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
10/02/10	S.Granet EDF-R&D/AMA	Initial version