
Models of Summarized behavior

THHM:

This note introduces a family of constitutive laws THM for the saturated and unsaturated mediums. One described there the relations allowing to calculate the hydraulic and thermal quantities, by taking account of strong couplings between these phenomena and also with the mechanical strains. The relations presented here can be coupled with any mechanical constitutive law, subject making the assumption known as of the effective stresses of Bishop and that the mechanical constitutive law defines constant elastics (useful for the coupled terms). The purely mechanical part of the models is not presented.

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1 Introduction

We introduce here a family of constitutive laws `THM` for the saturated and unsaturated mediums. We describe the relations allowing to calculate the hydraulic and thermal quantities, by taking account of strong couplings between these phenomena and also with the mechanical strains. The relations presented here can be coupled with any mechanical constitutive law, subject making the assumption known as of the effective stresses of Bishop and that the mechanical constitutive law defines constant elastics (useful for the coupled terms). For this reason, the purely mechanical part of the models is not presented here.

The modelizations selected O lean on the presentation of the porous environments elaborate in particular by Coussy [bib1]. The behavior models are obtained from thermodynamic considerations and with arguments of homogenization which we do not present here, and who are entirely described in the document of P. Charles [bib2]. In the same way the general writing of the balance equations and conservation is not detailed, and one returns the reader to the documents [R5.03.01] [bib3] and [R7.01.10] [bib4], which contain definitions useful for the comprehension of this document.

Mechanics of porous media a very exhaustive collection of physical phenomena concerning to solids and the fluids gathers. It makes the assumption of a coupling between the mechanical evolutions of solids and the fluids, seen like continuums, with the hydraulic evolutions, which solve the problems of diffusion of fluids within walls or volumes, and the thermal evolutions.

Each component of the porous environment thus has a structural mechanics behavior, hydraulics and thermal. The theory tries to gather all these physical phenomena. Chemical phenomena (transformations of the components, reactions producing of components etc...), just as the radiological phenomena are not taken into account at this stage of the development of *Code_Aster*. The mechanical, hydraulic and thermal phenomena are taken into account or not according to the behavior called upon by the user in command `STAT_NON_LINE`, according to the following nomenclature:

Modelization	Phenomena taken into account
<code>KIT_H</code>	Hydraulics with a Mechanical,
<code>hydraulic</code>	unknown pressure <code>KIT_HM</code> with a Mechanical,
<code>hydraulic</code>	unknown pressure <code>KIT_HHM</code> with two unknown pressures
<code>KIT_THH</code>	Thermal, hydraulics with two unknown pressures
<code>KIT_THM</code>	Thermal, mechanics, hydraulics with a Thermal,
<code>mechanical</code>	, hydraulic unknown pressure <code>KIT_THHM</code> with two unknown pressures

the document present describes the models for the most general case said `THHM`. The simpler cases are obtained starting from the general case by simply cancelling the quantity absent.

2 Presentation of problem: Assumptions, Notations

In this chapter, one mainly sticks to show the porous environment and its characteristics.

2.1 Description of the porous environment

the porous environment considered is a volume made up of a more or less homogeneous solid matrix, more or less coherent (very coherent in the case of the concrete, little in the case of sand). Between the solid elements, one finds pores. One distinguishes the closed pores which do not exchange anything with their neighbors and the connected pores in which the exchanges are numerous. When one speaks about porosity, it is well of these connected pores about which one speaks.

Inside these pores a certain number of fluids are (one excludes solidification from these fluids), present possibly under several phases (liquidates or gas exclusively), and presenting an interface with the other components. To simplify the problem and to take into account the relative importance of the physical phenomena, the only interface considered is that between the fluid and the gas, the interfaces solid fluid/being neglected.

2.2 Notations

We suppose that the pores of solid are occupied by with more the two components, each one coexistent in two phases to the maximum, one liquidates and the other gas one. The quantities X associated with the phase j ($j=1,2$) with the fluid i will be noted: X_{ij} . When there are two components besides solid, they are a fluid (typically water) and a gas (typically dry air), knowing that liquidates it can be present in gas form (vapor) in the gas mixture and that the air can be present in form dissolved in water. When there is one component besides solid, that can be a fluid or a gas. Thereafter one will speak about air for the gas component, but it can be a question of any other composing (hydrogen, CO_2 etc).

The porous environment at current time is noted Ω , its border $\partial\Omega$. It is noted $\Omega_0, \partial\Omega_0$ at initial time.

The medium is defined by:

- parameters (vector position x , time t),
- variables (displacements, pressures, temperature),
- quantities intrinsic (forced and mass strains, contributions, heat, enthalpy, flux hydraulic, thermals...).

The general assumptions carried out are the following ones:

- assumption of small displacements,
- reversible thermodynamic evolutions (not necessarily for the mechanics),
- isotropic behavior,
- the gases are perfect gases,
- mixes ideal perfect gases (stagnation pressure = sum of the partial pressures),
- thermodynamic equilibrium between the phases of the same component.

The various notations are clarified hereafter.

2.2.1 Descriptive variables of the medium

These are the variables whose knowledge according to time and of the place make it possible to know the state of the medium completely. These variables break up into two categories:

- geometrical, variable

- variables of thermodynamic state.

2.2.1.1 Geometrical variables

In all that follows, one adopts a Lagrangian representation compared to the squelette (within the meaning of [bib1]) and the coordinated $\mathbf{x} = \mathbf{x}_s(t)$ are those of a material point attached to the squelette. All the spatial derivative operators are defined compared to these coordinates.

Displacements of the squelette are noted $\mathbf{u}(\mathbf{x}, t) = \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}$.

2.2.1.2 Variables of thermodynamic state

In a general way, the following indices are used:

- w for liquid water,
- ad the dissolved air,
- as the dry air,
- vp the steam.

The thermodynamic variables are:

- pressures of the components: $p_w(\mathbf{x}, t)$ $p_{ad}(\mathbf{x}, t)$ $p_{vp}(\mathbf{x}, t)$ $p_{as}(\mathbf{x}, t)$,
- the temperature of the medium: $T(\mathbf{x}, t)$.

These various variables are not completely independent. Indeed, if only one component is considered, the thermodynamic equilibrium between its phases imposes a relation between the steam pressure and the pressure of the fluid 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.

For the case known as saturated (only one component air or water) we chose the pressure of this single constituting.

For the case says unsaturated (presence of air and water), we chose like independent variables:

- stagnation pressure of gas: $p_{gz}(\mathbf{x}, t) = p_{vp} + p_{as}$,
- capillary pressure: $p_c(\mathbf{x}, t) = p_{gz} - p_{lq} = p_{gz} - p_w - p_{ad}$.

These pressures have a very strong physical interpretation, the total gas pressure for obvious reasons, and the capillary pressure, also called suction, because the capillary phenomena are very important in the modelization presented here. It would have been possible also to choose the steam pressure or the percentage of relative moisture (relationship between the steam pressure and the saturating steam pressure) physically accessible. The modelization becomes more complex then and in any event, capillary pressure, gas pressure and percentage of relative moisture (relationship between the steam pressure and the saturating steam pressure) are connected by the model of Kelvin.

For the cas particulier of the behavior "LIQU_GAZ_ATM" one says makes the assumption known as of Richards: the pores are not saturated by the fluid, but the pressure of gas is supposed to be constant and the only variable of pressure is the fluid pressure.

2.2.1.3 Descriptive fields of the medium

the principal unknowns, who are also the nodal unknowns (noted $\mathbf{U}(\mathbf{x}, t)$ in this document) are:

- 2 or 3 (according to the dimension of space) displacements $u_x(\mathbf{x}, t), u_y(\mathbf{x}, t), u_z(\mathbf{x}, t)$ for modelizations `KIT_HM`, `KIT_HHM`, `KIT_THM`, `KIT_THHM`,
- the temperature $T(\mathbf{x}, t)$ for modelizations `KIT_THH`, `KIT_THM`, `KIT_THHM`,
- two pressures $p_1(\mathbf{x}, t), p_2(\mathbf{x}, t)$ (which are $p_c(\mathbf{x}, t), p_{gz}(\mathbf{x}, t)$ in the case studied) for modelizations `KIT_HHM`, `KIT_THH`, `KIT_THHM`,
- a pressure $p_1(\mathbf{x}, t)$ (which is $p_w(\mathbf{x}, t)$ or $p_{gz}(\mathbf{x}, t)$ according to whether the medium is saturated by a fluid or a gas) for modelizations `KIT_H`, `KIT_HM`, `KIT_THM`.

2.2.2 Particulate derivatives

This paragraph shows the paragraph partly “derived particulate, voluminal and mass densities” of the document [R7.01.10]. Description that we make of the medium is Lagrangian compared to the squelette.

Either a an unspecified field on Ω , or $\mathbf{x}_s(t)$ the punctual coordinate attached to the squelette that we follow in his motion and or $\mathbf{x}_f(t)$ the punctual coordinate attached to the fluid. One notes

$\dot{a} = \frac{d^s a}{dt}$ temporal derivative in the motion of the squelette:

$$\dot{a} = \frac{d^s a}{dt} = \lim_{\Delta t \rightarrow 0} \frac{a(\mathbf{x}(t+\Delta t), (t+\Delta t)) - a(\mathbf{x}(t), t)}{\Delta t}$$

\dot{a} is called particulate and often noted derivative $\frac{da}{dt}$. We prefer to use a notation which recalls that the configuration used to locate a particle is that of the squelette compared to which a fluid particle has a relative velocity. For a fluid particle the location $\mathbf{x}_s(t)$ is unspecified, i.e. that the fluid particle which occupies the position $\mathbf{x}_s(t)$ at time t is not the same one as that which occupies the position $\Omega^0(1+\varepsilon_v)(1-\varphi) = \Omega^0(1-\varphi^0)(1+\varepsilon_{v_s})$ at another time t' .

2.2.3 Quantities

the balance equations are:

- conservation of the linear momentum for the mechanics,
- the conservation lots of fluid for the hydraulics,
- the conservation of energy for the thermal.

The writing of these equations is given in the document [R7.01.10] [bib4], which defines also what we call in a general way a constitutive law `THM` and gives the definitions of the stresses and generalized strains. This document uses these definitions. The balance equations utilize directly the generalized stresses.

The generalized stresses are connected to the strains generalized by the constitutive laws. The generalized strains are calculated directly starting from the variables of state and their temporal spatial gradients.

The constitutive laws can use additional quantities, often arranged in the local variables. We gather here under the term of quantity at the same time the stresses, the strains and of the additional quantities.

2.2.3.1 Quantities characteristic of the heterogeneous medium

- eulerian porosity: φ .

If one notes $\Omega_{(\varphi)}$ the part of the volume Ω occupied by the vacuums in the current configuration, one a:

$$\varphi = \frac{\Omega_{(\varphi)}}{\Omega}$$

the definition of porosity is thus that of eulerian porosity.

- Fluid saturation: S_{lq}

If one notes Ω_{lq} the total volume occupied by the fluid, in the current configuration, one has by definition:

$$S_{lq} = \frac{\Omega_{lq}}{\Omega_{\varphi}}$$

This saturation is thus finally a proportion varying between 0 and 1.

- Eulerian densities of water ρ_w , the dissolved air ρ_{ad} , the dry air ρ_{as} , the vapor ρ_{vp} , gas ρ_{gz} .

If one notes γ_w (resp γ_{ad} γ_{as} , γ_{vp}) the masses of water (resp of dissolved air, dry air and vapor) contents in a volume of Ω the squelette in the current configuration, one has by definition:

$$\begin{aligned} \gamma_w &= \int_{\Omega} \rho_w S_{lq} \varphi d \Omega & \gamma_{ad} &= \int_{\Omega} \rho_{ad} S_{lq} \varphi d \Omega \\ \gamma_{as} &= \int_{\Omega} \rho_{as} (1 - S_{lq}) \varphi d \Omega & \gamma_{vp} &= \int_{\Omega} \rho_{vp} (1 - S_{lq}) \varphi d \Omega \end{aligned}$$

The density of the gas mixture is simply the sum of the densities of the dry air and the vapor:

$$\rho_{gz} = \rho_{as} + \rho_{vp}$$

In the same way for the liquid mixture:

$$\rho_{lq} = \rho_w + \rho_{ad}$$

One notes ρ_w^0 , ρ_{ad}^0 , ρ_{vp}^0 , ρ_{as}^0 the initial values of the densities.

- Lagrangian homogenized density: r .

To time running the mass of volume Ω M_{Ω} , is given by: $M_{\Omega} = \int_{\Omega_0} r d \Omega_0$.

2.2.3.2 Mechanical magnitudes

- the tensor of the strains $\boldsymbol{\varepsilon}(\mathbf{u})(\mathbf{x}, t) = \frac{1}{2}(\nabla \mathbf{u} + {}^T \nabla \mathbf{u})$.

One will note $\epsilon_V = \text{tr}(\boldsymbol{\varepsilon})$.

- The tensor of the stresses which are exerted on the porous environment: $\boldsymbol{\sigma}$.

This tensor breaks up into a tensor of the effective stresses plus a stress tensor of pressure $\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \sigma_p \mathbf{I}$ and σ_p are of the components generalized stresses . This cutting is finally

rather arbitrary, but corresponds all the same to an assumption rather commonly allowed, at least for the mediums saturated with fluid.

2.2.3.3 Hydraulic quantities

- mass contributions in components $m_w, m_{ad}, m_{vp}, m_{as}$ (unit: kilogram per cubic meter). They represent the mass of fluid brought between initial and current times. They belong to the generalized stresses.
- Hydraulic flux $\mathbf{M}_w, \mathbf{M}_{ad}, \mathbf{M}_{vp}, \mathbf{M}_{as}$ (unit: kilogram/second/square meter). One could not give very well no more precise definition of the contributions of mass and flux, considering that their definition is summarized to check the balance equations hydraulics:

$$\begin{cases} \dot{m}_w + \dot{m}_{vp} + \text{Div}(\mathbf{M}_w + \mathbf{M}_{vp}) = 0 \\ \dot{m}_{as} + \dot{m}_{ad} + \text{Div}(\mathbf{M}_{as} + \mathbf{M}_{ad}) = 0 \end{cases} \quad \text{éq 2.2.3.3 - 1}$$

We nevertheless will specify the physical meaning as of these quantities, knowing that what we write now is already a constitutive law.

The velocities of the components are measured in a fixed reference frame in space and time.

One notes \mathbf{v}_w the velocity of water, \mathbf{v}_{ad} that of the dissolved air, \mathbf{v}_{vp} that of the vapor,

\mathbf{v}_{as} that of the dry air, and $\mathbf{v}_s = \frac{d\mathbf{u}}{dt}$ that of the squelette.

The mass contributions are defined by:

$$\begin{aligned} m_w &= \rho_w (1 + \varepsilon_V) \varphi S_{lq} - \rho_w^0 \varphi^0 S_{lq}^0 \\ m_{ad} &= \rho_{ad} (1 + \varepsilon_V) \varphi S_{lq} - \rho_{ad}^0 \varphi^0 S_{lq}^0 \\ m_{as} &= \rho_{as} (1 + \varepsilon_V) \varphi (1 - S_{lq}) - \rho_{as}^0 \varphi^0 (1 - S_{lq}^0) \\ m_{vp} &= \rho_{vp} (1 + \varepsilon_V) \varphi (1 - S_{lq}) - \rho_{vp}^0 \varphi^0 (1 - S_{lq}^0) \end{aligned} \quad \text{éq 2.2.3.3 - the 2}$$

mass flux are defined by:

$$\begin{aligned} \mathbf{M}_w &= \rho_w \varphi S_l (\mathbf{v}_w - \mathbf{v}_s) \\ \mathbf{M}_{ad} &= \rho_{ad} \varphi S_l (\mathbf{v}_{ad} - \mathbf{v}_s) \\ \mathbf{M}_{as} &= \rho_{as} \varphi (1 - S_l) (\mathbf{v}_{as} - \mathbf{v}_s) \\ \mathbf{M}_{vp} &= \rho_{vp} \varphi (1 - S_l) (\mathbf{v}_{vp} - \mathbf{v}_s) \end{aligned} \quad \text{éq 2.2.3.3 - the 3}$$

mass contributions make it possible to define the total density seen compared to the reference configuration:

$$r = r_0 + m_w + m_{ad} + m_{vp} + m_{as} \quad \text{éq 2.2.3.3 - 4}$$

where r_0 the density homogenized at initial time indicates.

Other intermediate hydraulic quantities are introduced:

- concentration of the vapor in gas: $C_{vp} = \frac{p_{vp}}{p_{gz}}$,
- gas flux: $\frac{\mathbf{M}_{gz}}{\rho_{gz}} = (1 - C_{vp}) \frac{\mathbf{M}_{as}}{\rho_{as}} + C_{vp} \frac{\mathbf{M}_{vp}}{\rho_{vp}}$. This equation specifies that the velocity of gas is obtained by making an average (balanced sum) velocities of various gases according to their concentration,
- the steam pressure p_{vp} .

2.2.3.4 Thermal quantities

- not convectée heat Q' (see further) (unit: Joule),
- mass enthalpy of the components h_{ij}^m ($h_w^m, h_{ad}^m, h_{vp}^m, h_{as}^m$) (unit: Joule/Kelvin/kilogram),
- heat flux: \mathbf{q} (unit: $J/s/m^2$).

All these quantities belong to the generalized stresses within the meaning of the document [R7.01.10] [bib4].

2.2.4 External data

- the mass force \mathbf{F}^m (in practice gravity),
- heat sources Θ ,
- boundary conditions relating either to variables imposed, or on imposed flux.

3 Constitutive equations

3.1 Conservation equations

It is here only about one recall, the way of establishing them is presented in [R7.01.10] [bib4].

3.1.1 Balance mechanical

By noting $\boldsymbol{\sigma}$ the tensor of the total mechanical stresses and r the homogenized density of the medium, the mechanical equilibrium is written:

$$\text{Div}(\boldsymbol{\sigma}) + r \mathbf{F}^m = \mathbf{0} \quad \text{éq 3.1.1-1}$$

We point out that r is connected to the variations of fluid mass by the relation:

$$r = r_0 + m_w + m_{ad} + m_{vp} + m_{as} \quad \text{éq 3.1.1-2}$$

3.1.2 Conservation of the fluid masses

For the fluid the derivative $\dot{a} = \frac{d^s a}{dt}$ is in fact an eulerian derivative and the equations which we write for the fluid comprise of the terms of transport, even if they can be hidden by the choice of the unknowns. The conservation equations of the fluid masses are written then:

$$\begin{cases} \dot{m}_w + \dot{m}_{vp} + Div(M_w + M_{vp}) = 0 \\ \dot{m}_{as} + \dot{m}_{ad} + Div(M_{as} + M_{ad}) = 0 \end{cases} \quad \text{éq 3.1.2-1}$$

3.1.3 Conservation of energy: thermal equation

$$\begin{aligned} h_w^m \dot{m}_w + h_{ad}^m \dot{m}_{ad} + h_{vp}^m \dot{m}_{vp} + h_{as}^m \dot{m}_{as} + \dot{Q}' + Div(h_w^m \mathbf{M}_w + h_{ad}^m \mathbf{M}_{ad} + h_{vp}^m \mathbf{M}_{vp} + h_{as}^m \mathbf{M}_{as}) + Div(\mathbf{q}) = \\ (\mathbf{M}_w + \mathbf{M}_{ad} + \mathbf{M}_{vp} + \mathbf{M}_{as}) F^m + \Theta \end{aligned} \quad \text{éq 3.1.3-1}$$

3.2 Equations of behavior

3.2.1 Evolution of porosity

3.2.1.1 general Case

$$d\varphi = (b - \varphi) \left(d\varepsilon_V - 3\alpha_0 dT + \frac{dp_{gz} - S_{lq} dp_c}{K_s} \right) \quad \text{éq 3.2.1-1}$$

In this equation, one sees appearing the coefficients b and K_s . b is the coefficient of Biot and K_s is the modulus of compressibility of the solid matter constituents. If K_0 the modulus of compressibility "drained" of the porous environment indicates, there is the relation:

$$b = 1 - \frac{K_0}{K_s} \quad \text{éq 3.2.1-2}$$

Note:

Statement 3.2.1-1 can appear unusual taking into account the standard definition of the coefficient of Biot. That is due to the fact that we use eulerian porosity φ whereas the usual definition of the coefficient of Biot is based on the Lagrangian definition Φ of this quantity.

The two definitions are connected by the relation:

$$\Phi = (1 + \varepsilon_V) \varphi \quad \text{éq 3.2.1-3}$$

In the case of an isothermal evolution for a saturated medium, the variation of Lagrangian porosity is simply proportional to the variation of volume:

$$d\Phi = b \cdot d\varepsilon_V \quad \text{éq 3.2.1-4}$$

Deferring éq 3.2.1-4 in éq 3.2.1-3, one finds:

$$(1 + \varepsilon_V) d\varphi = (b - \varphi) d\varepsilon_V$$

For ε_V small (assumption retained in modelizations THM), one obtains $d\varphi = (b - \varphi) d\varepsilon_V$, who corresponds well to [éq 3.2.1-1] for the examined case.

3.2.1.2 Case without mechanical coupling

For the purely hydraulic or thermohydraulic modelizations without mechanical coupling, it is however possible to vary porosity via a coefficient of storage E_m . This last then connects the variation of porosity to the variation of fluid pressure such as:

$$d\varphi = E_m dp_{lq}$$

This coefficient is not taken into account in the case of the modelizations with mechanics (*HM*)

3.2.2 Evolution of the contributions of fluid mass

By means of the definition of the contributions of fluid mass and while putting forward purely geometrical arguments, one finds:

$$\begin{aligned} m_w &= \rho_w (1 + \varepsilon_V) \varphi S_{lq} - \rho_w^0 \varphi^0 S_{lq}^0 \\ m_{ad} &= \rho_{ad} (1 + \varepsilon_V) \varphi S_{lq} - \rho_{ad}^0 \varphi^0 S_{lq}^0 \\ m_{as} &= \rho_{as} (1 + \varepsilon_V) \varphi (1 - S_{lq}) - \rho_{as}^0 \varphi^0 (1 - S_{lq}^0) \\ m_{vp} &= \rho_{vp} (1 + \varepsilon_V) \varphi (1 - S_{lq}) - \rho_{vp}^0 \varphi^0 (1 - S_{lq}^0) \end{aligned} \quad \text{éq 3.2.2-1}$$

Note: .

If we use Lagrangian porosity, the contributions mass would be written:

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

As example, we show the first relation in the saturated case $S_{lq} = 1$ (with $\rho_{lq} = \rho_w$).

That is to say an elementary field of porous environment of volume Ω . One notes Ω_s the volume occupied by the solid matter constituents and Ω_l the volume occupied by the fluid and gas. One notes Ω^0 , Ω_s^0 , Ω_l^0 same volumes in an initial state. We point out that ε_V note the variation of volume of the porous environment and we note ε_{Vs} the voluminal variation of the solid matter constituents.

One has by definition: $\varphi = \frac{\Omega_l}{\Omega}$

$$\Omega_s = \Omega - \Omega_l = \Omega (1 - \varphi) = \Omega_s^0 (1 + \varepsilon_{Vs})$$

But $\Omega (1 - \varphi) = \Omega^0 (1 + \varepsilon_V) (1 - \varphi)$.

One from of deduced:

$$\Omega^0 (1 + \varepsilon_V) (1 - \varphi) = \Omega_s^0 (1 + \varepsilon_{Vs})$$

It is enough to write then $\Omega_s^0 = \Omega^0 (1 - \varphi^0)$ to obtain:

$$\Omega^0 (1 + \varepsilon_V) (1 - \varphi) = \Omega^0 (1 - \varphi^0) (1 + \varepsilon_{Vs})$$

From where one deduces:

$$\varepsilon_{Vs} (1 - \varphi^0) = \varepsilon_V (1 - \varphi) - (\varphi - \varphi^0)$$

One uses the eulerian definition of the homogenized density r' (not to be confused with the Lagrangian definition of the equation [éq 3.1.1-2]):

$$r' = \rho_{(s)} (1 - \varphi) + \rho_{(lq)} \varphi$$

and the definition of the mass fluid contribution:

$$r' \Omega = (r_0 + m_{lq}) \Omega^0$$

One obtains:

$$\rho_s (1 - \varphi) \Omega + \rho_{lq} \varphi \Omega = \rho_{s}^0 (1 - \varphi^0) \Omega^0 + \rho_{lq}^0 \varphi^0 \Omega^0 + m_{lq} \Omega^0$$

that is to say still:

$$\rho_s \Omega_s + \rho_{lq} \varphi (1 + e_V) \Omega^0 = \rho_s^0 \Omega_s^0 + \rho_{lq}^0 \varphi^0 \Omega^0 + m_{lq} \Omega^0$$

Using the conservation of the mass of the solid matter constituents: $\rho_s \Omega_s = \rho_s^0 \Omega_s^0$ one obtains finally:

$$\rho_{lq} \varphi (1 + \varepsilon_V) = \rho_{lq}^0 \varphi^0 + m_{lq}$$

3.2.3 Constitutive laws of the fluids

3.2.3.1 Liquid

$$\frac{d \rho_w}{\rho_w} = \frac{dp_w}{K_w} - 3 \alpha_w dT \quad \text{éq 3.2.3.1 - 1}$$

One sees appearing the modulus of compressibility of water K_w and its modulus of thermal expansion α_w .

3.2.3.2 Gas

For the equations of reaction of gases, one takes the model of perfect gases:

$$\frac{p_{vp}}{\rho_{vp}} = \frac{R}{M_{vp}^{ol}} T \quad \text{éq 3.2.3.2 - 1}$$

$$\frac{p_{as}}{\rho_{as}} = \frac{R}{M_{as}^{ol}} T \quad \text{éq 3.2.3.2 - 2}$$

One sees appearing the molar mass of the vapor M_{vp}^{ol} , and that of the dry air M_{as}^{ol} .

3.2.4 Evolution of the enthalpy

3.2.4.1 liquid Enthalpy

$$dh_w^m = C_w^p dT + (1 - 3 \alpha_w T) \frac{dp_w}{\rho_w} \quad \text{éq 3.2.4.1 - 1}$$

One sees appearing the specific heat with constant pressure of water: C_w^p .

By replacing in this statement the pressure of the fluid by his value according to the capillary pressure and of the pressure of gas, one a:

$$dh_w^m = \left(1 - 3\alpha_w T\right) \frac{dp_{gz} - dp_c - dp_{ad}}{\rho_w} + C_w^p dT \quad \text{éq 3.2.4.1 - 2}$$

By noting C_{ad}^p the specific heat with constant pressure of the dissolved air, one a:

$$dh_{ad}^m = C_{ad}^p dT \quad \text{éq 3.2.4.1 - 3}$$

3.2.4.2 Enthalpy of the gases

$$dh_{vp}^m = C_{vp}^p dT \quad \text{éq 3.2.4.2 - 1}$$

$$dh_{as}^m = C_{as}^p dT \quad \text{éq 3.2.4.2 - 2}$$

One sees appearing the specific heat with constant pressure of the dry air C_{as}^p and that of the vapor C_{vp}^p .

3.2.4.3 Contribution of heat except fluids

It is the quantity $\delta Q'$ which represents the heat received by the system except contribution enthalpic of the fluids.

$$\delta Q' = 3\alpha_0 K_0 T d\varepsilon_V + 3\alpha_{lq}^m T dp_c - \left(3\alpha_{gz}^m + 3\alpha_{lq}^m\right) T dp_{gz} + C_\varepsilon^0 dT \quad \text{éq 3.2.4.3 - 1}$$

One sees appearing several coefficients of thermal expansion: $\alpha_0, \alpha_{lq}^m, \alpha_{gz}^m$. The coefficient α_0 is a data: it corresponds at the same time to the coefficient of thermal expansion of the porous environment and that of the solid matter constituents (which are being inevitably equal in the theory that we present here).

$\alpha_{lq}^m, \alpha_{gz}^m$ are given by the relations:

$$\alpha_{gz}^m = \left(1 - S_{lq}\right) (b - \varphi) \alpha_0 + \frac{\varphi (1 - S_{lq})}{3T} \quad \text{éq 3.2.4.3 - 2}$$

$$\alpha_{lq}^m = S_{lq} (b - \varphi) \alpha_0 + \alpha_{lq} \varphi S_{lq} \quad \text{éq 3.2.4.3 - 3}$$

One also sees appearing in [éq 3.2.4.3 - 1] the specific heat with constant strain of the porous environment C_ε^0 , which depends on the specific heat with constant stress of the porous environment C_σ^0 by the relation:

$$C_\varepsilon^0 = C_\sigma^0 - 9TK_0 \alpha_0^2 \quad \text{éq 3.2.4.3 - 4}$$

C_σ^0 is given by a model of mixture:

$$C_\sigma^0 = \left(1 - \varphi\right) \rho_s C_\sigma^s + S_{lq} \varphi \left(\rho_w C_w^p + \rho_{ad} C_{ad}^p\right) + \varphi \left(1 - S_{lq}\right) \left(\rho_{vp} C_{vp}^p + \rho_{as} C_{as}^p\right) \quad \text{éq 3.2.4.3 - 5}$$

where C_σ^s represents the specific heat with constant stress of the solid matter constituents and ρ_s the density of the solid matter constituents. For the computation of ρ_s , one neglects the strain of the

solid matter constituents, one thus confuses ρ_s with his initial value ρ_s^0 , which is calculated in fact from the initial specific mass of the porous environment r_0 by the following formula of the mixtures:

$$(1 - \varphi^0) \rho_s^0 = r_0 - (\rho_w^0 + \rho_{ad}^0) S_{lq}^0 \varphi^0 - \varphi^0 (1 - S_{lq}^0) (\rho_{vp}^0 + \rho_{as}^0) \quad \text{éq 3.2.4.3 - 6}$$

3.2.5 Models of diffusion (complementary models)

3.2.5.1 Diffusion of heat

One takes the classical model of Fourier:

$$\mathbf{q} = -\lambda^T \cdot \nabla T \quad \text{éq 3.2.5.1 - 1}$$

where one sees appearing the thermal coefficient of conductivity λ^T .

λ^T is function of porosity, saturation and temperature and is given in the shape of the product of three functions plus a constant:

$$\lambda^T = \lambda_\varphi^T(\phi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) + \lambda_{cte}^T \quad \text{éq 3.2.5.1 - 2}$$

3.2.5.2 Diffusion of the fluids

They are the models of Darcy, to which one adds the model of Fick in the presence of vapor. The models of Darcy are written for gas and the fluid:

$$\frac{\mathbf{M}_{lq}}{\rho_{lq}} = \lambda_{lq}^H (-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m) \quad \text{éq 3.2.5.2 - 1}$$

$$\frac{\mathbf{M}_{gz}}{\rho_{gz}} = \lambda_{gz}^H (-\nabla p_{gz} + \rho_{gz} \mathbf{F}^m) \quad \text{éq 3.2.5.2 - 2}$$

where we see appearing hydraulic conductivities λ_{lq}^H and λ_{gz}^H for the fluid and gas respectively.

One makes the approximation that $\frac{\mathbf{M}_w}{\rho_w} = \lambda_w^H (-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m)$.

The diffusion in the gas mixture is given by the model of Fick thanks to the relation:

$$\frac{\mathbf{M}_{vp}}{\rho_{vp}} - \frac{\mathbf{M}_{as}}{\rho_{as}} = -\frac{D_{vp}}{C_{vp}(1 - C_{vp})} \nabla \left(\frac{p_{vp}}{p_{gz}} \right) \quad \text{éq 3.2.5.2 - 3}$$

where D_{vp} is the coefficient of diffusion of Fick of the gas mixture (L2.T-1), one notes by the suitetel F_{vp} that:

$$F_{vp} = \frac{D_{vp}}{C_{vp}(1 - C_{vp})} \quad \text{éq 3.2.5.2 - 4}$$

and with

$$C_{vp} = \frac{P_{vp}}{P_{gz}} \quad \text{éq 3.2.5.2 - 5}$$

One thus has:

$$\frac{\mathbf{M}_{vp}}{\rho_{vp}} - \frac{\mathbf{M}_{as}}{\rho_{as}} = -F_{vp} \nabla C_{vp} \quad \text{éq 3.2.5.2 - 6}$$

Moreover, one a:

$$\frac{\mathbf{M}_{gz}}{\rho_{gz}} = (1 - C_{vp}) \frac{\mathbf{M}_{as}}{\rho_{as}} + C_{vp} \frac{\mathbf{M}_{vp}}{\rho_{vp}} \quad \text{éq 3.2.5.2 - 7}$$

and:

$$\rho_{gz} = \rho_{vp} + \rho_{as} \quad \text{éq 3.2.5.2 - 8}$$

For the diffusion of the liquid mixture, the usual writing is the following one:

$$\mathbf{M}_{ad} - \mathbf{M}_w = -D_{ad} \nabla \rho_{ad} \quad \text{éq 3.2.5.2 - 9}$$

where D_{ad} is the coefficient of diffusion of Fick of the liquid mixture. In order to keep a homogeneous writing with that of the gas mixture one notes by the suitetel F_{ad} that:

$$F_{ad} = D_{ad} \quad \text{éq 3.2.5.2 - 10}$$

And the concentration C_{ad} corresponds here to the density of the dissolved air:

$$C_{ad} = \rho_{ad} \quad \text{éq 3.2.5.2 - 11}$$

$$\mathbf{M}_{ad} - \mathbf{M}_w = -F_{ad} \nabla C_{ad} \quad \text{éq 3.2.5.2 - 12}$$

Concerning the fluid, one admitted that the liquid model of Darcy applies at the speed of liquid water. There is not thus to define mean velocity of the fluid.

$$\frac{\mathbf{M}_w}{\rho_w} = \lambda_{lq}^H \left(-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m \right) \quad \text{éq 3.2.5.2 - 13}$$

and:

$$\rho_{lq} = \rho_w + \rho_{ad} \quad \text{éq 3.2.5.2 - 14}$$

By combining these relations, one find then:

$$\frac{\mathbf{M}_{as}}{\rho_{as}} = \lambda_{gz}^H \left(-\nabla p_{gz} + \rho_{gz} \mathbf{F}^m \right) + C_{vp} F_{vp} \nabla C_{vp} \quad \text{éq 3.2.5.2 - 15}$$

$$\frac{\mathbf{M}_{vp}}{\rho_{vp}} = \lambda_{gz}^H \left(-\nabla p_{gz} + \rho_{gz} \mathbf{F}^m \right) - (1 - C_{vp}) F_{vp} \nabla C_{vp} \quad \text{éq 3.2.5.2 - 16}$$

$$\frac{\mathbf{M}_w}{\rho_w} = \lambda_{lq}^H \left(-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m \right) \quad \text{éq 3.2.5.2 - 17}$$

$$\mathbf{M}_{ad} = \rho_{ad} \lambda_{lq}^H \left(-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m \right) - F_{ad} \nabla C_{ad} \quad \text{éq 3.2.5.2 - 18}$$

hydraulic conductivities λ_{lq}^H and λ_{gz}^H are not directly data and their value is known starting from the formulas:

$$\lambda_{lq}^H = \frac{K^{\text{int}}(\varphi) \cdot k_{lq}^{\text{rel}}(S_{lq})}{\mu_w(T)} \quad \text{éq 3.2.5.2 - 19}$$

$$\lambda_{gz}^H = \frac{K^{\text{int}}(\varphi) \cdot k_{gz}^{\text{rel}}(S_{lq}, p_{gz})}{\mu_{gz}(T)} \quad \text{éq 3.2.5.2 - 20}$$

K^{int} is the intrinsic permeability, characteristic of the porous environment and user datum, unspecified function of porosity;

μ_w is the dynamic viscosity of water, characteristic of water and user datum, unspecified function of the temperature;

μ_{gz} is the dynamic viscosity of gas, characteristic of gas and user datum, unspecified function of the temperature;

k_{lq}^{rel} is the permeability relating to the fluid, characteristic of the porous environment and user datum, unspecified function of fluid saturation;

k_{gz}^{rel} is the permeability relating to gas, characteristic of the porous environment and user datum, unspecified function of fluid saturation and gas pressure.

Note:

Here definite hydraulic conductivities are not inevitably very familiar for the mechanics of soils, which usually use for the saturated mediums the permeability k , which is homogeneous at a velocity.

The relation enters k and λ_{lq}^H is as follows: $\lambda_{lq}^H = \frac{k}{\rho_w g}$ where g is the acceleration of gravity.

The coefficient of diffusion of Fick of the gas mixture F_{vp} is a characteristic of the porous environment, unspecified user datum function of the steam pressure, gas pressure, saturation and temperature which one will write like a product of function of each one of these variables:

$F_{vp}(P_{vp}, P_{gz}, T, S) = f_{vp}^{vp}(P_{vp}) \cdot f_{vp}^{gz}(P_{gz}) \cdot f_{vp}^T(T) \cdot f_{vp}^S(S)$ one will neglect derivatives compared to the steam pressure and saturation. Same way for the coefficient of diffusion of Fick of the liquid medium: $F_{ad}(P_{ad}, P_{lq}, T, S) = f_{ad}^{ad}(P_{ad}) \cdot f_{ad}^{lq}(P_{lq}) \cdot f_{ad}^T(T) \cdot f_{ad}^S(S)$, one takes into account only derivative according to the temperature.

3.2.6 Water-steam equilibrium

This relation is essential and it results in to reduce the number of unknowns of pressure.

One notes h_w^m the mass enthalpy of water, s_w^m his entropy and $g_w^m = h_w^m - Ts_w^m$ his free enthalpy.

One notes h_{vp}^m the mass enthalpy of the vapor, s_{vp}^m his entropy and $g_{vp}^m = h_{vp}^m - Ts_{vp}^m$ his free enthalpy.

The equilibrium water vapor is written:

$$g_{vp}^m = g_w^m \quad \text{éq 3.2.6-1}$$

Which gives:

$$h_{vp}^m - h_w^m = T (s_{vp}^m - s_w^m) \quad \text{éq 3.2.6-2}$$

In addition, the definition of the free enthalpy teaches us that: $dg = \frac{dp}{\rho} - sdT$, which, applied to the vapor and water, compound with the relation $dg_{vp}^m = dg_w^m$ and by means of [éq 3.2.6-2] gives:

$$\frac{dp_{vp}}{\rho_{vp}} = \frac{dp_w}{\rho_w} + (h_{vp}^m - h_w^m) \frac{dT}{T} \quad \text{éq 3.2.6-3}$$

This relation can be expressed according to the capillary pressure and of the gas pressure:

$$dp_{vp} = \frac{\rho_{vp}}{\rho_w} (dp_{gz} - dp_c - dp_{ad}) + \rho_{vp} (h_{vp}^m - h_w^m) \frac{dT}{T} \quad \text{éq 3.2.6-4}$$

3.2.7 Equilibrium air dissolved dryness-air

the dissolved air is defined via the constant of Henry K_H , who connects the molar concentration of dissolved air C_{ad}^{ol} (moles/m³) to the air pressure dryness:

$$C_{ad}^{ol} = \frac{p_{as}}{K_H} \quad \text{éq 3.2.7-1}$$

$$\text{with } C_{ad}^{ol} = \frac{\rho_{ad}}{M_{ad}^{ol}} \quad \text{éq 3.2.7-2}$$

the molar mass of the dissolved air, M_{ad}^{ol} is logically the same one as that of the dry air M_{as}^{ol} . For the dissolved air, one takes the model of perfect gas:

$$\frac{p_{ad}}{\rho_{ad}} = \frac{R}{M_{as}^{ol}} T \quad \text{éq 3.2.7-3}$$

the dissolved air pressure is thus connected to that of dry air by:

$$p_{ad} = \frac{p_{as}}{K_H} RT \quad \text{éq 3.2.7-4}$$

3.2.8 the structural mechanics behavior

One will write it in differential form:

$$d\sigma = d\sigma' + d\sigma_p \mathbf{I} \quad \text{éq 3.2.8-1}$$

By means of a formulation of Bishop [bib10] extended to the unsaturated mediums one writes:

Warning : The translation process used on this website is a "Machine Translation". It may be imprecise and inaccurate in whole or in part and is provided as a convenience.

$$d \sigma_p = -b(dp_{gz} - S_{lq} dp_c) \quad \text{éq 3.2.8-2}$$

In the relation [éq 3.2.8-1] the effective evolution of the stress tensor σ' is supposed to depend only on the displacement of the squelette and the local variables α . The usual terms related to the thermal strain are integrated into the computation of the effective stress:

$$d \sigma' = f(d \epsilon - \alpha_0 dT \mathbf{I}, d \alpha) \quad \text{éq 3.2.8-3}$$

the reason of this choice is to be able to use any model of classical thermomechanics for the computation of the effective stresses, models which, in more the share of the writings are in conformity with [éq 3.2.8-3].

3.2.9 Precise details on the diphasic terms of transfers

3.2.9.1 the isotherm of sorption

to close the system, it remains still a relation to be written, connecting saturation and the pressures. We chose to consider that fluid saturation was an unspecified function of the capillary pressure, that this function was a characteristic of the porous environment and provided in data by the user.

Since the user can provide a function closely connected very $S_{lq}(p_c)$ well per pieces, and since the

derivative of this function $\frac{\partial S_{lq}}{\partial p_c}$, plays an essential physical role, we chose to require of the user to

also provide this curve, remainder with its load to make sure of the coherence of the data thus specified. There exists however for the user the possibility of calling on an analytical model of saturation and its derivative coded "into tough" in the source: the model of Mualem-Van Genuchten (see following section).

It is noticed that in the approach present, one speaks about a bi-univocal relation between saturation and capillary pressure. It is known that for most porous environments, it is not the same relation which must be used for the paths of drying and the paths of hydration. It is one of the limits of the approach present.

3.2.9.2 The model Mualem - Van Genuchten

Concerning the hydraulic behavior, the user currently has two choices: to return manually, and in tabulated form, relative permeabilities, models of saturation and their derivatives while making sure of their coherence (key word `HYDR_UTIL` under `RELATION_KIT`), is to call on a model known and programmed in analytical form: the model Mualem - Van Genuchten (key word `HYDR_VGM` or `HYDR_VGC` under `RELATION_KIT`).

Note:

There exists of course of other classical models to describe the hydraulic behavior (Brook Corey for example) but it are currently not available in Aster. It is then to the user to return them in tabulated form in the command file. The model Mualem- Van Genuchten is a classical model for the description of the typical argillaceous materials of the problems of storage under ground. For the permeability relating to gas, it is current to use either a version Van Genuchten, or a cubic version.

The model Mualem-Van Genuchten results in a model capillary saturation/pressure (Van Genuchten) such as:

$$S_{we} = \frac{1}{\left[1 + \left(\frac{P_c}{P_r} \right)^n \right]^m}$$

$$\text{with } S_{we} = \frac{S - S_{wr}}{1 - S_{wr}} \text{ and } m = 1 - \frac{1}{n}$$

n , S_{wr} (residual water saturation) and P_r are parameters of the models indicated by the user in his command file.

The permeability relating to water is expressed then by integrating the model prediction proposed by Mualem (1976) in the model of capillarity of Van Genuchten:

$$k_r^w = \sqrt{S_{we}} \left(1 - \left(1 - S_{we}^{1/m} \right)^m \right)^2$$

The permeability with gas is formulated in a similar way in the case of the model HYDR_VGM:

$$k_r^{gz} = \sqrt{\left(1 - S_{we} \right)} \left(1 - S_{we}^{1/m} \right)^{2m}$$

or by a simple cubic model in the case of the HYDR_VGC:

$$k_r^{gz} = \left(1 - S \right)^3$$

In *Code_Aster*, we make a digital processing of this model in the "limiting" zones ($S=1$ or $S=0$). For that we use two additional parameters corresponding to a processing which one carries out on these curves, S_{max} and $CSAT$:

For $S > S_{max}$, these curves are interpolated by a polynomial of degree 2 CI in S_{max} , so as to avoid having to treat derivatives of infinite values. Indeed, for $S=1$:

$$\frac{\partial k_r^w(S)}{\partial S} = \infty$$

and for case HYDR_VGM $\frac{\partial k_r^{gz}(S)}{\partial S} = \infty$

to avoid having then to deal with this problem (which does not have a priori physical meaning) one replaces these functions from a saturation S_{max} by a polynomial of the second order CI in this point.

What gives for the function $k_r^w(S)$:

For $S = S_{max}$, one determines the polynomial $PL(S)$ such as:

$$\begin{cases} PL(S_{max}) = k_r^w(S_{max}) \\ PL'(S_{max}) = \frac{\partial k_r^w}{\partial S}(S_{max}) \end{cases} \text{ and } PL(1) = 0$$

For $S > S_{max}$, $k_r^w(S)$ par. And $PL(S)$

for in $k_r^{gz}(S)$ case HYDR_VGM is replaced:

For $S = S_{max}$, one determines the polynomial $PG(S)$ such as:

$$\begin{cases} PG(S_{max}) = k_r^{gz}(S_{max}) \\ PG'(S_{max}) = \frac{\partial k_r^{gz}}{\partial S}(S_{max}) \end{cases} \text{ and } PG(0) = 1$$

For $S > S_{max}$, $k_r^{gz}(S)$ par. For $PG(S)$

suction is replaced $S(P_c)$ and for $P_c < P_{cmin}$ (with $S(P_{cmin}) = S_{max}$) one prolongs the curve $S(P_c)$ by a hyperbole such as the curve is CI in this point:

For $S > S_{max}$:

$$S(P_c) = 1 - \frac{A}{B - P_c}$$

with A and B such as the curve is CI in S_{max} .

There is thus well a decreasing curve which tends towards 1 when P_c tends towards $-\infty$. This processing enables us to manage negative capillary pressures (in these zones there the terms of capillary pressure is abusive, it acts implicitly of a change of variable making it possible to deal with a quasi-saturated problem).

$S(P_c)$ is then multiplied by a coefficient "of security" $CSAT$ so that the saturation never reaches 1 (problem which one cannot treat). One advises to take a value of $CSAT$ very near to 1 (0,999999 for example).

3.2.10 Summary of the characteristics of the material and the user data

- the Young's modulus E_0 and the drained Poisson's ratio ν_0 make it possible to calculate the modulus of compressibility drained of the porous environment by $K_0 = \frac{E_0}{3(1 - 2\nu_0)}$,
- the coefficient of Biot $b = 1 - \frac{K_0}{K_s}$ makes it possible to calculate the modulus of compressibility of the solid matter constituents K_s ,
- the modulus of compressibility of water K_w ,
- the coefficient of thermal expansion of water α_w ,
- the constant of perfect gases R ,
- the molar mass of the vapor M_{vp}^{ol} ,
- the molar mass of the dry air $M_{as}^{ol} (= M_{ad}^{ol})$,
- the specific heat with constant pressure of water C_w^p ,
- the specific heat with constant pressure of the dissolved air C_{ad}^p ,
- the specific heat with constant pressure of the dry air C_{as}^p ,
- the specific heat with constant pressure of the vapor C_{vp}^p ,
- the coefficient of thermal expansion of the porous environment α_0 which is also that of the solid matter constituents,
- the specific heat with constant stress of the solid matter constituents C_{σ}^s ,
- the coefficient of thermal conductivity of the solid matter constituents only λ_s^T , unspecified function of the temperature,
- the coefficient of thermal conductivity of the fluid λ_{lq}^T , unspecified function of the temperature,
- the coefficient of thermal conductivity of the dry air λ_{as}^T , unspecified function of the temperature,
- the coefficient of diffusion of Fick for the gas mixture F_{vp} , unspecified function of the temperature, the gas pressure, the steam pressure and saturation
- the coefficient of diffusion of Fick for the liquid mixture F_{ad} , unspecified function of the fluid temperature and pressure, pressure of the dissolved air and saturation.

- The constant of unspecified K_H Henry function of the temperature,
- the intrinsic permeability K^{int} , unspecified function of porosity,
- the dynamic viscosity of water μ_w , unspecified function of the temperature,
- the dynamic viscosity of gas μ_{gz} , unspecified function of the temperature,
- the permeability relating to the fluid k_{lq}^{rel} , unspecified function of fluid saturation,
- the permeability relating to gas k_{gz}^{rel} , unspecified function of fluid saturation and the gas pressure,
- the relation capillary saturation/pressure $S_{lq}(p_c)$, unspecified function of the capillary pressure,
- a general way the initial state is characterized by:
 - the initial temperature,
 - initial pressures from where initial saturation is deduced $S_{lq}^0(p_c^0)$,
 - the initial specific mass of water ρ_w^0 ,
 - initial porosity φ^0 ,
 - initial pressure of the vapor p_{vp}^0 from where one deduces the initial density from the vapor ρ_{vp}^0 ,
 - initial pressure of the dry air p_{as}^0 from where one deduces the initial density from L`dry air ρ_{as}^0 .
 - homogenized initial density porous environment r_0 ,
 - initial enthalpi of water, dissolved air, vapor and dry air.

3.3 The state of reference and the initial state

the introduction of the initial conditions is very important, in particular for the enthalpi. In practice, one can reason by considering that one has three states for the fluids:

- the state running,
- the state of reference: it is that of the fluids in a free state. Very often one will take for the pressures of water and air the atmospheric pressure. In this state of reference, one can consider that the enthalpi are null,
- the initial state: it is important to note that, in an initial state of the porous environment, water is in a hygroscopic state different from that of free water. For the enthalpi of water and vapor one will have to take:

$$\begin{aligned} {}^{init} h_w^m &= \frac{p_w^{init} - p_l^{ref}}{\rho_w} = \frac{p_w^{init} - p_{atm}}{\rho_w} \\ {}^{init} h_{vp}^m &= L(T^{init}) = \text{chaleur latente de vaporisation} \\ {}^{init} h_{as}^m &= 0 \\ {}^{init} h_{ad}^m &= 0 \end{aligned}$$

Note:

The initial vapor pressure must be taken in coherence with the other data. Very often, one leaves the knowledge of an initial state of hygroscopy. The relative humidity is the relationship between the steam pressure and the steam pressure saturating with the temperature considered. One then uses the model of Kelvin which gives the pressure of the fluid according to the steam pressure, of the temperature and the saturating steam pressure: $\frac{p_w - p_w^{ref}}{\rho_w} = \frac{R}{M_{ol}^{vp}} T \ln\left(\frac{p_{vp}}{p_{vp}^{sat}(T)}\right)$. This relation is valid only for isothermal

evolutions. It is stressed that p_w^{ref} corresponds in a state of "equilibrium to which corresponds p_{vp}^{sat} , this state D" equilibrium corresponds in fact to $p_w^0 = p_{gz}^0 = 1 \text{ atm}$. For evolutions with temperature variation, knowing a model giving the steam pressure saturating to the temperature T_0 , for example:

$$p_{vp}^{sat}(T_0) = 10^{\left(\frac{2.7858 + \frac{T_0 - 273.5}{31.559 + 0.1354(T_0 - 273.5)}} \right)}$$

and a degree of hygroscopy HR , one from of deduced the steam pressure thanks to $p_{vp}(T_0) = HR p_{vp}^{sat}(T_0)$.

3.4 Nodal unknowns, initial values and values of reference

We approach here a point which is due more to choices of programming than to true aspects of formulation. Nevertheless, we expose it because it has important practical consequences. The principal unknowns who are also the values of the degrees of freedom, are noted:

$$\{u\}^{ddl} = \begin{pmatrix} u_x \\ u_y \\ u_z \\ \text{PRE1}^{ddl} \\ \text{PRE2}^{ddl} \\ T^{ddl} \end{pmatrix}$$

According to the modelization, they can have different meanings:

	LIQU_SATU	LIQU_VAPE	LIQU_GAZ_ATM	GAZ	LIQU_VAPE_GAZ
PRE1	p_w	p_w	$p_c = -p_w$	p_{gz}	$p_c = p_{gz} - p_w$
PRE2					p_{gz}

	LIQU_GAZ	LIQU_AD_GAZ_VAPE	LIQU_AD_GAZ
PRE1	$p_c = p_{gz} - p_w$	$p_c = p_{gz} - p_w - p_{ad}$	$p_c = p_{gz} - p_w - p_{ad}$
PRE2	p_{gz}	p_{gz}	p_{gz}

One will then define the real pressures and the real temperature by:

$p = p^{ddl} + p^{init}$ for pressures PRE1 and PRE2 and $T = T^{ddl} + T^{init}$ the temperatures, where p^{init} and T^{init} are defined under key word THM_INIT of the command DEFI_MATERIAU.

The values written by IMPR_RESU are the values of $\{u\}^{ddl}$. The boundary conditions are defined for $\{u\}^{ddl}$. Key word DEPL of the key word factor ETAT_INIT of the command STAT_NON_LINE defines the initial values of $\{u\}^{ddl}$. Initial values of the enthalpi, which belong to the generalized stresses are defined starting from key word SIGM of the key word factor ETAT_INIT of the command STAT_NON_LINE. The real pressures and the real temperature are used in the constitutive laws, in

particular the models of the type $S_{iq} = f(p_c)$ or $\frac{dp}{p} = \frac{d\rho}{\rho} + \frac{dT}{T}$. The initial values of the densities

of the vapor and the dry air are defined starting from the initial values of the vapor and gas pressures (values read under key word THM_INIT of the command DEFI_MATERIAU). It is noticed that, for displacements, decomposition $u = u^{ddl} + u^{init}$ is not made: key word THM_INIT of the command DEFI_MATERIAU thus does not make it possible to define initial displacements. The only way of

initializing displacements is thus to give them an initial value by the key word factor `ETAT_INIT` of the command `STAT_NON_LINE`.

3.5 Total effective stresses and stresses. Boundary conditions of stress

the partition of the stresses in stresses total and effective is written:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \sigma_p \mathbf{I}$$

$\boldsymbol{\sigma}$ is the total stress, i.e. that which checks: $\text{Div}(\boldsymbol{\sigma}) + r \mathbf{F}^m = \mathbf{0}$

$\boldsymbol{\sigma}'$ is the effective stress. For the models of effective stresses, it checks: $d\boldsymbol{\sigma}' = f(d\boldsymbol{\varepsilon} - \alpha_0 dT, \boldsymbol{\alpha})$, where $\boldsymbol{\varepsilon} = 1/2(\nabla \mathbf{u} + {}^T \nabla \mathbf{u})$ and $\boldsymbol{\alpha}$ represents the local variables.

σ_p is calculated according to the water pressures. Writing adopted is incremental and, if it is wanted that the value of σ_p is coherent with the value p^{init} defined under key word `THM_INIT`, he is necessary to initialize σ_p by key word `SIGM` of the key word factor `ETAT_INIT` of the command `STAT_NON_LINE`.

In results files, one finds the effective stresses $\boldsymbol{\sigma}'$ under the names of components `SIXX ...` and σ_p under name `SIP`. The boundary conditions in stresses are written in total stresses.

3.6 Some numerical values

We give here some reasonable values for certain coefficients. These values are not programmed in `Code_Aster`, they are provided here as an indication:

For perfect gases, one retains the following values:

$$\begin{aligned} R &= 8.3144 \text{ J} \cdot \text{K}^{-1} \\ M_{vp}^{ol} &= 18.10^{-3} \text{ kg} \cdot \text{mole}^{-1} \\ M_{as}^{ol} &= 28.9610^{-3} \text{ kg} \cdot \text{mole}^{-1} \end{aligned}$$

For CO2, the value of the constant of Henry with 20°C is of:

$$K_H = 3162 \text{ Pa} \cdot \text{m}^3 \text{mole}^{-1}$$

For liquid water, one a:

$$\begin{aligned} \rho_w &= 1000 \text{ kg/m}^3 \\ K_w &= 2000 \text{ MPa} \end{aligned}$$

the thermal coefficient of thermal expansion of water is correctly approached by the formula:

$$\alpha_w = 9.52 \cdot 10^{-5} \ln(T - 273) - 2.19 \cdot 10^{-4} \text{ (K}^{-1}\text{)}$$

Heat capacities have as values:

$$\begin{aligned} C_\sigma^s &= 800 \text{ J} \cdot \text{kg}^{-1} \text{K}^{-1} \\ C_{lq}^p &= 4180 \text{ J} \cdot \text{kg}^{-1} \text{K}^{-1} \\ C_{vp}^p &= 1870 \text{ J} \cdot \text{kg}^{-1} \text{K}^{-1} \\ C_{as}^p &= 1000 \text{ J} \cdot \text{kg}^{-1} \text{K}^{-1} \end{aligned}$$

To a law of evolution of the latent heat of liquid phase change vapor is also given:

$$L(T) = 2500800 - 2443(T - 273.15) \text{ J/kg}$$

4 Computation of the generalized stresses

In this chapter, we specify how are integrated the relations described into chapter 3. More precisely still, we give the statements of the generalized stresses within the meaning of the document [R7.01.10] [bib4] when constitutive laws THM are called for the option RAPH_MECA within the meaning of the document [R5.03.01] [bib3]. So that this document follows of reader the order of programming, we will consider two cases: the case without dissolved air and that with.

The generalized stresses are:

$$\boldsymbol{\sigma}', \sigma_p; m_w, \mathbf{M}_w, h_w^m; m_{vp}, \mathbf{M}_{vp}, h_{vp}^m; m_{as}, \mathbf{M}_{as}, h_{as}^m; m_{ad}, \mathbf{M}_{ad}, h_{ad}^m; \mathbf{Q}', \mathbf{q}$$

The generalized strains, from which the generalized stresses are calculated are:

$$\mathbf{u}, \boldsymbol{\varepsilon}(\mathbf{u}); p_c, \nabla p_c; p_{gz}, \nabla p_{gz}; T, \nabla T$$

The local variables which we retained are:

- In the case without vapor:

$$\varphi, \rho_w, S_{lq}$$

- In the case with vapor and without dissolved air:

$$\varphi, \rho_w, p_{vp}, S_{lq}$$

- In the case with dissolved vapor and air:

$$\varphi, \rho_w, p_{vp}, p_{ad}, S_{lq}$$

In this chapter, we adopt the usual notations Aster, namely the indices + for the values of the quantities at the end of time step and the indices - for the quantities at the beginning of time step.

Thus, the known quantities are:

- generalized stresses, strains and local variables at the beginning of time step:
 - $\boldsymbol{\sigma}'^-, \sigma_p^-; m_w^-, \mathbf{M}_w^-, h_w^{m^-}; m_{vp}^-, \mathbf{M}_{vp}^-, h_{vp}^{m^-}; m_{as}^-, \mathbf{M}_{as}^-, h_{as}^{m^-}; m_{ad}^-, \mathbf{M}_{ad}^-, h_{ad}^{m^-}; \mathbf{Q}'^-, \mathbf{q}^-$
 - $\mathbf{u}^-, \boldsymbol{\varepsilon}(\mathbf{u}^-); p_c^-, \nabla p_c^-; p_{gz}^-, \nabla p_{gz}^-; T^-, \nabla T^-$
 - $\varphi^-, \rho_w^-, p_{vp}^-, p_{ad}^-$
- strains generalized at the end of time step:
 - $\mathbf{u}^+, \boldsymbol{\varepsilon}(\mathbf{u}^+); p_c^+, \nabla p_c^+; p_{gz}^+, \nabla p_{gz}^+; T^+, \nabla T^+$
- The unknown quantities are the stresses, and local variables at the end of time step:
 - $\boldsymbol{\sigma}'^+, \sigma_p^+; m_w^+, \mathbf{M}_w^+, h_w^{m^+}; m_{vp}^+, \mathbf{M}_{vp}^+, h_{vp}^{m^+}; m_{as}^+, \mathbf{M}_{as}^+, h_{as}^{m^+}; m_{ad}^+, \mathbf{M}_{ad}^+, h_{ad}^{m^+}; \mathbf{Q}'^+, \mathbf{q}^+$
 - $\varphi^+, \rho_w^+, p_{vp}^+, p_{ad}^+$

4.1 Case without dissolved air

4.1.1 Computation of porosity and its density of the fluid

the first thing to be made is of course to calculate saturation at the end of time step $S_{lq}^+ = S_{lq}(p_c^+)$. Porosity is while integrating on time step the equation [eq 3.2.1-1].

One obtains then:

$$\ln \left(\frac{b - \varphi^+}{b - \varphi^-} \right) = \left(-(\varepsilon_v^+ - \varepsilon_v^-) + 3 \alpha_0 (T^+ - T^-) - \frac{(p_{gz}^+ - p_{gz}^-) - S_{lq}^+ (p_c^+ - p_c^-)}{K_s} \right) \quad \text{éq 4.1.1-1}$$

the density of the fluid is while integrating on time step the equation [éq 3.2.3.1 - 1].

What gives:

$$\ln \left(\frac{\rho_w^+}{\rho_w^-} \right) = \frac{p_{gz}^+ - p_{gz}^- - p_c^+ + p_c^-}{K_w} - 3 \alpha_w (T^+ - T^-) \quad \text{éq 4.1.1-2}$$

4.1.2 Computation of the coefficients of thermal expansion

It acts of a simple application of the formulas [éq 3.2.4.3 - 2] and [éq 3.2.4.3 - 3], which are evaluated at the end of time step:

$$\alpha_{vp}^{m^+} = \alpha_{as}^{m^+} = \alpha_{gz}^{m^+} = (1 - S_{lq}^+) (b - \varphi^+) \alpha_0 + \frac{\varphi^+ (1 - S_{lq}^+)}{3 T^+} \quad \text{éq 4.1.2-1}$$

$$\alpha_w^{m^+} = S_{lq}^+ (b - \varphi^+) \alpha_0 + \alpha_{lq} \varphi^+ S_{lq}^+ \quad \text{éq 4.1.2-2}$$

4.1.3 Computation of the fluid enthalpi

the fluid enthalpi are calculated by integration of the equations [éq 3.2.4.1 - 1], [éq 3.2.4.2 - 1], [éq 3.2.4.2 - 2].

$$h_w^{m^+} = h_w^{m^-} + C_w^p (T^+ - T^-) + \frac{(1 - 3 \alpha_w T^+)}{\rho_w^+} (p_{gz}^+ - p_{gz}^- - p_c^+ + p_c^-) \quad \text{éq 4.1.3-1}$$

$$h_{vp}^{m^+} = h_{vp}^{m^-} + C_{vp}^p (T^+ - T^-) \quad \text{éq 4.1.3-2}$$

$$h_{as}^{m^+} = h_{as}^{m^-} + C_{as}^p (T^+ - T^-) \quad \text{éq 4.1.3-3}$$

4.1.4 Steam pressures and air

On the basis of the relation [éq 3.2.6-4] in which one carries the constitutive law of perfect gases [éq 3.2.3.2 - 1], one finds $\frac{dp_{vp}}{p_{vp}} = \frac{M^{ol}}{RT} \left(\frac{1}{\rho_w} dp_{gz} - \frac{1}{\rho_w} dp_c + (h_{vp}^m - h_w^m) \frac{dT}{T} \right)$ that one integrates by a path initially into constant temperature (one then considers the density of constant water), then of T^- with T^+ constant pressures.

$$\ln \left(\frac{p_{vp}^+}{p_{vp}^-} \right) = \frac{M^{ol}}{RT^+} \frac{1}{\rho_w^+} \left[(p_{gz}^+ - p_{gz}^-) - (p_c^+ - p_c^-) \right] + \frac{M^{ol}}{R} \int_{T^-}^{T^+} (h_{vp}^m - h_w^m) \frac{dT}{T^2}$$

The first term corresponds to the path with constant temperature, the second at the path with constant pressures. By means of the definitions [éq 3.2.4.1 - 1] and [éq 3.2.4.2 - 1] of the enthalpi, it is seen that for an evolution with constant pressures:

$$\frac{h_{vp}^m - h_w^m}{T^2} = \frac{h_{vp}^{m'} - h_w^{m'}}{T^2} + \frac{(C_{vp}^p - C_w^p)(T - T^-)}{T^2}$$

One thus has for such a path:

$$\int_{T^-}^{T^+} (h_{vp}^m - h_w^m) \frac{dT}{T^2} = (h_{vp}^{m'} - h_w^{m'}) \left(\frac{1}{T^-} - \frac{1}{T^+} \right) + (C_{vp}^p - C_w^p) \left(\ln \left(\frac{T^+}{T^-} \right) + T^- \left(\frac{1}{T^+} - \frac{1}{T^-} \right) \right)$$

That is to say finally:

$$\ln \left(\frac{p_{vp}^+}{p_{vp}^-} \right) = \frac{M_{vp}^{ol}}{RT^+} \frac{1}{\rho_w^+} \left[(p_{gz^+} - p_{gz^-}) - (p_{c^+} - p_{c^-}) \right] + \frac{M_{vp}^{ol}}{R} (h_{vp}^{m'} - h_w^{m'}) \left(\frac{1}{T^-} - \frac{1}{T^+} \right) + \frac{M_{vp}^{ol}}{R} (C_{vp}^p - C_w^p) \left(\ln \left(\frac{T^+}{T^-} \right) + \frac{T^-}{T^+} - 1 \right) \quad \text{éq 4.1.4-1}$$

One can then calculate the densities of the vapor and the air by the relations [éq 3.2.3.2 - 1] and [éq 3.2.3.2 - 2]:

$$\rho_{vp}^+ = \frac{M_{vp}^{ol}}{R} \frac{p_{vp}^+}{T^+} \quad \text{éq 4.1.4-2}$$

$$\rho_{as}^+ = \frac{M_{as}^{ol}}{R} \frac{(p_{gz^+} - p_{vp}^+)}{T^+} \quad \text{éq 4.1.4-3}$$

4.1.5 Computation of the mass contributions

the equations [éq 3.2.2-1] give null mass contributions to time 0. One writes in an incremental way the equations [éq 3.2.2-1]:

$$\begin{aligned} m_w^+ &= m_w^- + \rho_w^+ (1 + \varepsilon_V^+) \varphi^+ S_{lq}^+ - \rho_w^- (1 + \varepsilon_V^-) \varphi^- S_{lq}^- \\ m_{as}^+ &= m_{as}^- + \rho_{as}^+ (1 + \varepsilon_V^+) \varphi^+ (1 - S_{lq}^+) - \rho_{as}^- (1 + \varepsilon_V^-) \varphi^- (1 - S_{lq}^-) \\ m_{vp}^+ &= m_{vp}^- + \rho_{vp}^+ (1 + \varepsilon_V^+) \varphi^+ (1 - S_{lq}^+) - \rho_{vp}^- (1 + \varepsilon_V^-) \varphi^- (1 - S_{lq}^-) \end{aligned} \quad \text{éq 4.1.5-1}$$

4.1.6 Computation of heat capacity and heat Q'

One now has all the elements to apply at the end of time step the formula [éq 3.2.4.3 - 5]:

$$C_\sigma^{0+} = (1 - \varphi^+) \rho_s C_\sigma^s + S_{lq}^+ \varphi^+ \rho_w^+ C_w^p + (1 - S_{lq}^+) \varphi^+ (\rho_{vp}^+ C_{vp}^p + \rho_{as}^+ C_{as}^p) \quad \text{éq 4.1.6-1}$$

One uses of course [éq 3.2.4.3 - 4] who gives:

$$C_{\varepsilon}^{0+} = C_{\sigma}^{0+} - 9 T^+ K_0 \alpha_0^2 \quad \text{éq 4.1.6-2}$$

Although the variation of heat $\delta Q'$ is not a total differential, it is nevertheless licit to integrate it on time step and one obtains while integrating [éq 3.2.4.3 - 1].

$$Q'^+ = Q'^- + 3 \alpha_0 K_0 T^{1/2} (\varepsilon_V^+ - \varepsilon_V^-) + 3 \alpha_{lq}^{m+} T^{1/2} (p_c^+ - p_c^-) - (3 \alpha_{gz}^{m+} + 3 \alpha_{lq}^{m+}) T^{1/2} (p_{gz}^+ - p_{gz}^-) + C_{\varepsilon}^{0+} (T^+ - T^-) \quad \text{éq 4.1.6-3}$$

where we noted: $T^{1/2} = \frac{T^+ + T^-}{2}$. We chose here a formula of "point medium" for the variable temperature.

4.1.7 Computation of the mechanical stresses

The computation of the effective stresses is done by calling upon the incremental models of mechanics chosen by the user. One integrates on time step [the éq 3.2.8-2] and one a:

$$\sigma_p^+ = \sigma_p^- - b (p_{gz}^+ - p_{gz}^-) + b S_{lq}^+ (p_c^+ - p_c^-) \quad \text{éq 4.1.7-1}$$

4.1.8 Computation of hydrous and thermal flux

It is of course necessary to calculate all the coefficients of diffusion:

- The coefficient of Fick $F^+ = F(T^+, p_c^+, p_{gz}^+)$
- thermal diffusivity $\lambda^{T+} = \lambda_{\phi}^T(\varphi^+) \cdot \lambda_S^T(S_{lq}^+) \cdot \lambda_T^T(T^+) + \lambda_{cte}^T$
- hydraulic permeabilities and conductivities:

$$\lambda_{lq}^{H+} = \frac{K^{int}(\varphi^+) \cdot k_w^{rel}(S_{lq}^+)}{\mu_w(T^+)} \quad \lambda_{gz}^{H+} = \frac{K^{int}(\varphi^+) \cdot k_{gz}^{rel}(S_{lq}^+, p_{gz}^+)}{\mu_{gz}(T^+)}$$

Vapor concentration: $C_{vp}^+ = \frac{p_{vp}^+}{p_{vp}^+}$

It does not remain any more whereas to apply the formulas [éq 3.2.5.1 - 1], [éq 3.2.5.2 - 15], [éq 3.2.5.2 - 16] and [éq 3.2.5.2 - 17] to find:

$$\mathbf{q}^+ = -\lambda^{T+} \nabla T^+ \quad \text{éq 4.1.8-1}$$

$$\frac{\mathbf{M}_{as}^+}{\rho_{as}^+} = \lambda_{gz}^{H+} \left[-\nabla p_{gz}^+ + (\rho_{as}^+ + \rho_{vp}^+) \mathbf{F}^m \right] + C_{vp}^+ F_{vp}^+ \nabla C_{vp}^+ \quad \text{éq 4.1.8-2}$$

$$\frac{\mathbf{M}_{vp}^+}{\rho_{vp}^+} = \lambda_{gz}^{H+} \left[-\nabla p_{gz}^+ + (\rho_{as}^+ + \rho_{vp}^+) \mathbf{F}^m \right] - (1 - C_{vp}^+) F_{vp}^+ \nabla C_{vp}^+ \quad \text{éq 4.1.8-3}$$

$$\frac{\mathbf{M}_w^+}{\rho_w^+} = \lambda_{lq}^{H^+} \left[-\nabla p_{lq}^+ + \rho_w^+ \mathbf{F}^m \right] \quad \text{éq 4.1.8-4}$$

4.2 Cases with dissolved air

4.2.1 Computation of the porosity

In the same way, the first thing to be made is to calculate saturation at the end of time step $S_{lq}^+ = S_{lq}(p_c^+)$. Porosity is while integrating on time step the equation [éq 3.2.1-1]. It is thus pointed out that:

$$\ln \left(\frac{b - \varphi^+}{b - \varphi^-} \right) = \left(-(\varepsilon_v^+ - \varepsilon_v^-) + 3 \alpha_0 (T^+ - T^-) - \frac{(p_{gz}^+ - p_{gz}^-) - S_{lq}^+(p_c^+ - p_c^-)}{K_S} \right)$$

4.2.2 Computation of the coefficients of thermal expansion

It acts of a simple application of the formulas [éq 3.2.4.3 - 2] and [éq 3.2.4.3 - 3], which are evaluated at the end of time step:

$$\alpha_{vp}^{m^+} = \alpha_{as}^{m^+} = \alpha_{gz}^{m^+} = (1 - S_{lq}^+) (b - \varphi^+) \alpha_0 + \frac{\varphi^+ (1 - S_{lq}^+)}{3 T^+} \quad \text{éq 4.2.2-1}$$

$$\alpha_w^{m^+} = S_{lq}^+ (b - \varphi^+) \alpha_0 + \alpha_{lq} \varphi^+ S_{lq}^+ \quad \text{éq 4.2.2-2}$$

$$\alpha_{ad}^{m^+} = S_{lq}^+ (b - \varphi^+) \alpha_0 + \frac{\varphi^+ S_{lq}^+}{3 T^+} \quad \text{éq 4.2.2-3}$$

4.2.3 Computation of density and dissolved and dry air, steam pressures

On the basis of the relation [éq 3.2.6-4] in which one carries the constitutive law of perfect gases [éq 3.2.3.2 - 1], one finds:

$$\frac{dp_{vp}}{p_{vp}} = \frac{M_{vp}^{ol}}{RT} \left(\frac{1}{\rho_w} dp_w + (h_{vp}^m - h_w^m) \frac{dT}{T} \right) \quad \text{éq 4.2.3-1}$$

Contrary to the case without dissolved air p_w is not now known any more:

$$p_w = p_{lq} - p_{ad} = p_{gz} - p_c - \frac{RT}{K_H} p_{as} = p_{gz} - p_c - \frac{RT}{K_H} (p_{gz} - p_{vp})$$

thus:

$$dp_w = dp_{gz} - dp_c - \frac{RT}{K_H} (dp_{gz} - dp_{vp}) - \frac{R}{K_H} (p_{gz} - p_{vp}) dT \quad \text{éq 4.2.3-2}$$

One integrates [éq 4.2.3.1] while including there [éq 4.2.3.2] by a path initially into constant temperature (one then considers the density of constant water), then of T^- with T^+ constant pressures. With final one obtains:

$$\ln\left(\frac{p_{vp}^+}{p_{vp}^-}\right) = \frac{M_{vp}^{ol}}{\rho_w^-} \left(\frac{1}{RT^+} - \frac{1}{K_H}\right) (p_{gz^+} - p_{gz}^-) + \frac{M_{vp}^{ol}}{\rho_w^- K_H} (p_{vp^+} - p_{vp}^-) - \frac{M_{vp}^{ol}}{\rho_w^- RT^+} (p_{c^+} - p_c^-) + \frac{M_{vp}^{ol} R}{\rho_w^- K_H} (p_{vp^+} - p_{gz}^+) \ln\left(\frac{T^+}{T^-}\right) + \frac{M_{vp}^{ol}}{R} \int_{T^-}^{T^+} (h_{vp}^m - h_w^m) \frac{dT}{T^2}$$

éq 4.2.3-3

Contrary to the preceding case, one has here a nonlinear equation to solve. One will make for that a method of type corrector-predictor. One poses \tilde{p}_{vp} such as:

$$\ln\left(\frac{\tilde{p}_{vp}}{p_{vp}^-}\right) = \frac{M_{vp}^{ol}}{\rho_w^-} \left(\frac{1}{RT^+} - \frac{1}{K_H}\right) (p_{gz^+} - p_{gz}^-) - \frac{M_{vp}^{ol}}{\rho_w^- RT^+} (p_{c^+} - p_c^-) + \frac{M_{vp}^{ol}}{R} \int_{T^-}^{T^+} (h_{vp}^m - h_w^m) \frac{dT}{T^2}$$

éq 4.2.3-4

and thus

$$\tilde{p}_{vp} = p_{vp}^- \cdot \exp\left(\frac{M_{vp}^{ol}}{\rho_w^-} \left(\frac{1}{RT^+} - \frac{1}{K_H}\right) (p_{gz^+} - p_{gz}^-) - \frac{M_{vp}^{ol}}{\rho_w^- RT^+} (p_{c^+} - p_c^-) + \int_{T^-}^{T^+} (h_{vp}^m - h_w^m) \frac{dT}{T^2}\right)$$

éq 4.2.3-5

Moreover, as in the section [§4.1.4], one recalls that:

$$\int_{T^-}^{T^+} (h_{vp}^m - h_w^m) \frac{dT}{T^2} = (h_{vp}^m - h_w^m) \left(\frac{1}{T^-} - \frac{1}{T^+}\right) + (C_{vp}^p - C_w^p) \left(\ln\left(\frac{T^+}{T^-}\right) + T^- \left(\frac{1}{T^+} - \frac{1}{T^-}\right)\right)$$

Like $\ln\left(\frac{p_{vp}^+}{p_{vp}^-}\right) = \ln\left(\frac{\tilde{p}_{vp}}{p_{vp}^-}\right) + \ln\left(\frac{p_{vp}^+}{\tilde{p}_{vp}}\right)$ and that by D.L $\ln\left(\frac{p_{vp}^+}{\tilde{p}_{vp}}\right) = \ln\left(1 + \frac{p_{vp}^+ - \tilde{p}_{vp}}{\tilde{p}_{vp}}\right) \approx \frac{p_{vp}^+ - \tilde{p}_{vp}}{\tilde{p}_{vp}}$,

p_{vp}^+ will thus be given by the following linear statement:

$$\frac{p_{vp}^+}{\tilde{p}_{vp}} = 1 + \frac{M_{vp}^{ol}}{\rho_w^- K_H} (p_{vp^+} - p_{vp}^-) + \frac{M_{vp}^{ol} R}{\rho_w^- K_H} (p_{vp^+} - p_{gz}^-) \ln\left(\frac{T^+}{T^-}\right)$$

éq 4.2.3-6

from where

$$p_{vp}^+ = \frac{\left(\rho_w^- K_H - M_{vp}^{ol} \left(p_{vp}^- + p_{gz}^- R \ln\left(\frac{T^+}{T^-}\right)\right)\right)}{\left(\frac{\rho_w^- K_H}{\tilde{p}_{vp}} - M_{vp}^{ol} \left(1 + R \ln\left(\frac{T^+}{T^-}\right)\right)\right)}$$

éq 4.2.3-7

From there the other pressures is calculated easily:

$$p_{as}^+ = p_{gz}^+ - p_{vp}^+$$

$$p_{ad}^+ = \frac{P_{as}^+}{K_H} RT^+$$

$$p_w^+ = p_{gz}^+ - p_c^+ - p_{ad}^+$$

One can then calculate the densities of the vapor and the air by the relations [éq 3.2.3.2 - 1], [éq 3.2.3.2 - 2] and [éq 3.2.7-3]:

$$\rho_{vp}^+ = \frac{M_{vp}^{ol} p_{vp}^+}{R T^+} \quad \text{éq 4.2.3-8}$$

$$\rho_{as}^+ = \frac{M_{as}^{ol} (p_{gz}^+ - p_{vp}^+)}{R T^+} \quad \text{éq 4.2.3-9}$$

$$\rho_{ad}^+ = \frac{p_{ad}^+ M_{as}^{ol}}{RT^+} \quad \text{éq 4.2.3-10}$$

the density of water is while integrating on time step the equation [éq 3.2.3.1 - 1].

What gives:

$$\ln\left(\frac{\rho_w^+}{\rho_w^-}\right) = \frac{p_{gz}^+ - p_{gz}^- - p_c^+ + p_c^- - p_{ad}^+ + p_{ad}^-}{K_w} - 3\alpha_w(T^+ - T^-) \quad \text{éq 4.2.3-11}$$

4.2.4 Computation of the fluid enthalpi

the fluid enthalpi are calculated by integration of the equations [éq 3.2.4.1 - 1], [éq 3.2.4.1 - 3], [éq 3.2.4.2 - 1], [éq 3.2.4.2 - 2].

$$h_w^{m^+} = h_w^{m^-} + C_w^p(T^+ - T^-) + \frac{(1 - 3\alpha_w T^+)}{\rho_w^+} (p_{gz}^+ - p_{gz}^- - p_c^+ + p_c^- - p_{ad}^+ + p_{ad}^-) \quad \text{éq 4.2.4-1}$$

$$h_{ad}^{m^+} = h_{ad}^{m^-} + C_{ad}^p(T^+ - T^-) \quad \text{éq 4.2.4-2}$$

$$h_{vp}^{m^+} = h_{vp}^{m^-} + C_{vp}^p(T^+ - T^-) \quad \text{éq 4.2.4-3}$$

$$h_{as}^{m^+} = h_{as}^{m^-} + C_{as}^p(T^+ - T^-) \quad \text{éq 4.2.4-4}$$

4.2.5 Computation of the mass contributions

the equations [éq 3.2.2-1] give null mass contributions to time 0. One writes in an incremental way the equations [éq 3.2.2-1]:

$$\begin{aligned}
 m_w^+ &= m_w^- + \rho_w^+ (1 + \varepsilon_V^+) \varphi^+ S_{lq}^+ - \rho_w^- (1 + \varepsilon_V^-) \varphi^- S_{lq}^- \\
 m_{ad}^+ &= m_{ad}^- + \rho_{ad}^+ (1 + \varepsilon_V^+) \varphi^+ S_{lq}^+ - \rho_{ad}^- (1 + \varepsilon_V^-) \varphi^- S_{lq}^- \\
 m_{as}^+ &= m_{as}^- + \rho_{as}^+ (1 + \varepsilon_V^+) \varphi^+ (1 - S_{lq}^+) - \rho_{as}^- (1 + \varepsilon_V^-) \varphi^- (1 - S_{lq}^-) \\
 m_{vp}^+ &= m_{vp}^- + \rho_{vp}^+ (1 + \varepsilon_V^+) \varphi^+ (1 - S_{lq}^+) - \rho_{vp}^- (1 + \varepsilon_V^-) \varphi^- (1 - S_{lq}^-)
 \end{aligned}$$

éq 4.2.5-1

4.2.6 Computation of heat capacity and heat Q'

One now has all the elements to apply at the end of time step the formula [éq 3.2.4.3 - 5]:

$$C_\sigma^{0+} = (1 - \varphi^+) \rho_s C_\sigma^s + S_{lq}^+ \varphi^+ (\rho_w^+ C_w^p + \rho_{ad}^+ C_{ad}^p) + (1 - S_{lq}^+) \varphi^+ (\rho_{vp}^+ C_{vp}^p + \rho_{as}^+ C_{as}^p)$$

éq 4.2.6-1

One uses of course [éq 3.2.4.3 - 4] who gives:

$$C_\varepsilon^{0+} = C_\sigma^{0+} - 9 T^+ K_0 \alpha_0^2$$

éq 4.2.6-2

Although the variation of heat $\delta Q'$ is not a total differential, it is nevertheless licit to integrate it on time step and one obtains while integrating [éq 3.2.4.3 - 1].

$$Q'^+ = Q'^- + 3 \alpha_0 K_0 T^{1/2} (\varepsilon_V^+ - \varepsilon_V^-) + 3 \alpha_{lq}^{m^+} T^{1/2} (p_c^+ - p_c^-) - (3 \alpha_{gz}^{m^+} + 3 \alpha_{lq}^{m^+}) T^{1/2} (p_{gz}^+ - p_{gz}^-) + C_\varepsilon^{0+} (T^+ - T^-)$$

éq 4.2.6-3

where we noted: $T^{1/2} = \frac{T^+ + T^-}{2}$. We chose here a formula of "point medium" for the variable temperature.

4.2.7 Computation of the mechanical stresses

The computation of the effective stresses is done by calling upon the incremental models of mechanics chosen by the user. One integrates on time step [the éq 3.2.8-2] and one a:

$$\sigma_p^+ = \sigma_p^- - b (p_{gz}^+ - p_{gz}^-) + b S_{lq}^+ (p_c^+ - p_c^-)$$

éq 4.2.7-1

4.2.8 Computation of hydrous and thermal flux

It is of course necessary to calculate all the coefficients of diffusion:

Coefficients of Fick $F_{vp}^+(P_{vp}^+, P_{gz}^+, T^+, S^+)$ and $F_{ad}^+(P_{ad}^+, P_{lq}^+, T^+, S^+)$

thermal diffusivity $\lambda^{T^+} = \lambda_\varphi^T(\varphi^+) \cdot \lambda_S^T(S_{lq}^+) \cdot \lambda_T^T(T^+) + \lambda_{cte}^T$

hydraulic permeabilities and conductivities:

$$\lambda_{lq}^{H^+} = \frac{K^{\text{int}}(\varphi^+) \cdot k_w^{\text{rel}}(S_{lq}^+)}{\mu_w(T^+)} ; \lambda_{gz}^{H^+} = \frac{K^{\text{int}}(\varphi^+) \cdot k_{gz}^{\text{rel}}(S_{lq}^+, p_{gz}^+)}{\mu_{gz}(T^+)}$$

Concentrations out of vapor and dissolved air: $C_{vp}^+ = \frac{p_{vp}^+}{p_{gz}^+}$ and $C_{ad}^+ = \rho_{ad}^+$

It does not remain any more whereas to apply the formulas [éq 3.2.5.1 - 1], [éq 3.2.5.2 - 15], [éq 3.2.5.2 - 16], [éq 3.2.5.2 - 17] and [éq 3.2.5.2 - 18] to find:

$$\mathbf{q}^+ = -\lambda^{T^+} \nabla T^+ \quad \text{éq 4.2.8-1}$$

$$\frac{\mathbf{M}_{as}^+}{\rho_{as}^+} = \lambda_{gz}^{H^+} \left[-\nabla p_{gz}^+ + (\rho_{as}^+ + rh\delta_{vp}^+) \mathbf{F}^m \right] + C_{vp}^+ F_{vp}^+ \nabla C_{vp}^+ \quad \text{éq 4.2.8-2}$$

$$\frac{\mathbf{M}_{vp}^+}{\rho_{vp}^+} = \lambda_{gz}^{H^+} \left[-\nabla p_{gz}^+ + (\rho_{as}^+ + \rho_{vp}^+) \mathbf{F}^m \right] - (1 - C_{vp}^+) F_{vp}^+ \nabla C_{vp}^+ \quad \text{éq 4.2.8-3}$$

$$\frac{\mathbf{M}_w^+}{\rho_w^+} = \lambda_{lq}^{H^+} \left[-\nabla p_{lq}^+ + (\rho_w^+ + \rho_{ad}^+) \mathbf{F}^m \right] \quad \text{éq 4.2.8-4}$$

$$\mathbf{M}_{ad}^+ = \rho_{ad}^+ \lambda_{lq}^{H^+} \left[-\nabla p_{lq}^+ + (\rho_w^+ + \rho_{ad}^+) \mathbf{F}^m \right] - F_{ad}^+ \nabla C_{ad}^+ \quad \text{éq 4.2.8-5}$$

5 Computation of derivatives of the generalized stresses

In this chapter, we give the forms of derivatives of the generalized stresses compared to the strains generalized within the meaning of the document [R7.01.10] [bib4], C `be-with-to say the terms which are calculated when constitutive laws THM are called for the option RIGI_MECA_TANG within the meaning of the document [R5.03.01] [bib3].

In order not to weigh down the talk, we give the statement of the differentials of the generalized stresses, knowing that the partial derivatives result some directly.

5.1 Derived from the stresses

The computation of the differential of the effective stresses is left with the load of the purely mechanical constitutive law, which we do not describe in this document. The differential of the stress σ_p is given directly by the statement [éq 3.2.8-2].

5.2 Derived from the mass contributions

While differentiating [éq 3.2.2-1], one a:

$$\frac{dm_w}{\rho_w} = \frac{d\rho_w}{\rho_w} \left((1 + \varepsilon_V) \varphi S_{lq} + d\varepsilon_V \varphi S_{lq} + (1 + \varepsilon_V) d\varphi S_{lq} + (1 + \varepsilon_V) \varphi dS_{lq} \right)$$

$$\frac{dm_{ad}}{\rho_{ad}} = \frac{d\rho_{ad}}{\rho_{ad}} \left((1 + \varepsilon_V) \varphi S_{lq} + d\varepsilon_V \varphi S_{lq} + (1 + \varepsilon_V) d\varphi S_{lq} + (1 + \varepsilon_V) \varphi dS_{lq} \right)$$

$$\frac{dm_{as}}{\rho_{as}} = \frac{d\rho_{as}}{\rho_{as}} \left((1 + \varepsilon_V) \varphi (1 - S_{lq}) + d\varepsilon_V \varphi (1 - S_{lq}) + (1 + \varepsilon_V) d\varphi (1 - S_{lq}) - (1 + \varepsilon_V) \varphi dS_{lq} \right)$$

$$\frac{dm_{vp}}{\rho_{vp}} = \frac{d\rho_{vp}}{\rho_{vp}} \left((1 + \varepsilon_V) \varphi (1 - S_{lq}) + d\varepsilon_V \varphi (1 - S_{lq}) + (1 + \varepsilon_V) d\varphi (1 - S_{lq}) - (1 + \varepsilon_V) \varphi dS_{lq} \right)$$

éq 5.2-1

5.2.1 Cases without air dissolved

by taking account of [éq 3.2.1-1] and of [éq 3.2.3.1 - 1], [éq 3.2.3.2 - 1], [éq 3.2.3.2 - 2] and while supposing $1 + \varepsilon_V \approx 1$ one finds:

$$\left. \begin{aligned} \frac{dm_w}{\rho_w} &= b S_{lq} d\varepsilon_V + \left(\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{S_{lq} \varphi}{K_w} - \frac{S_{lq}^2 (b - \varphi)}{K_s} \right) dp_c + S_{lq} \left(\frac{\varphi}{K_w} + \frac{(b - \varphi)}{K_s} \right) dp_{gz} - 3 \alpha_w^m dT \\ \frac{dm_{vp}}{\rho_{vp}} &= b (1 - S_{lq}) d\varepsilon_V + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1 - S_{lq}) S_{lq} (b - \varphi)}{K_s} \right) dp_c + \left(\frac{(b - \varphi)(1 - S_{lq})}{K_s} \right) dp_{gz} + \varphi (1 - S_{lq}) \frac{dp_{vp}}{p_{vp}} - 3 \alpha_{vp}^m dT \\ \frac{dm_{as}}{\rho_{as}} &= b (1 - S_{lq}) d\varepsilon_V + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1 - S_{lq}) S_{lq} (b - \varphi)}{K_s} \right) dp_c + \left(\frac{(b - \varphi)(1 - S_{lq})}{K_s} \right) dp_{gz} + \varphi (1 - S_{lq}) \frac{dp_{as}}{p_{as}} - 3 \alpha_{as}^m dT \end{aligned} \right\}$$

éq 5.2.1-1

One sees compared to the appearing derivative of capillary fluid saturation pressure, quantity which plays a crucial role.

The statement [éq 3.2.6-4] of the differential of the steam pressure also makes it possible to calculate the air pressure dryness:

$$dp_{as} = \left(1 - \frac{M_{vp}^{ol} p_{vp}}{RT \rho_w} \right) dp_{gz} - \frac{M_{vp}^{ol}}{RT \rho_w} dp_c - \frac{M_{vp}^{ol}}{RT} \left(h_{vp}^m - h_w^m \right) \frac{dT}{T}$$

éq 5.2.1-2

One defers [éq 5.2.1-2] and [éq 3.2.6-4] in [éq 5.2.1-1] and one finds:

$$\frac{dm_w}{\rho_w} = bS_{lq} d\varepsilon_v + \left(\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{S_{lq}\varphi}{K_w} - \frac{S_{lq}^2(b-\varphi)}{K_s} \right) dp_c + S_{lq} \left(\frac{\varphi}{K_w} + \frac{(b-\varphi)}{K_s} \right) dp_{gz} - 3\alpha_w^m dT \quad \text{éq 5.2.1-3}$$

$$\begin{aligned} \frac{dm_{vp}}{\rho_{vp}} = & b(1-S_{lq}) d\varepsilon_v + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}(b-\varphi)}{K_s} - \frac{\varphi(1-S_{lq})\rho_{vp}}{p_{vp}\rho_{lq}} \right) dp_c \\ & + \left(\frac{(1-S_{lq})(b-\varphi)}{K_s} - \frac{\varphi(1-S_{lq})\rho_{vp}}{p_{vp}\rho_{lq}} \right) dp_{gz} \\ & + \left(-3\alpha_{vp}^m + \frac{\rho_{vp}\varphi(1-S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{vp}T} \right) dT \end{aligned} \quad \text{éq 5.2.1-4}$$

$$\begin{aligned} \frac{dm_{as}}{\rho_{as}} = & b(1-S_{lq}) d\varepsilon_v + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}(b-\varphi)}{K_s} - \frac{\varphi(1-S_{lq})\rho_{vp}}{p_{as}\rho_{lq}} \right) dp_c \\ & + \left(\frac{(1-S_{lq})(b-\varphi)}{K_s} - \frac{\varphi(1-S_{lq})\rho_{lq} - \rho_{vp}}{p_{as}\rho_{lq}} \right) dp_{gz} + \left(-3\alpha_{as}^m + \frac{\rho_{vp}\varphi(1-S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{as}T} \right) dT \end{aligned} \quad \text{éq 5.2.1-5}$$

5.2.2 Cases with air dissolved

Like previously, by taking account of [éq 3.2.1-1] and of [éq 3.2.3.1 - 1], [éq 3.2.3.2 - 1], [éq 3.2.3.2 - 2], [éq 3.2.7.3] and while supposing $1 + \varepsilon_v \approx 1$ one finds:

$$\begin{aligned} \frac{dm_w}{\rho_w} = & bS_{lq} d\varepsilon_v + \left(\frac{S_{lq}\varphi}{K_w} \frac{\partial p_w}{\partial P_c} - \frac{S_{lq}^2(b-\varphi)}{K_s} + \varphi \frac{\partial S_{lq}}{\partial P_c} \right) dp_c + S_{lq} \left(\frac{\varphi}{K_w} \frac{\partial p_w}{\partial P_{gz}} + \frac{(b-\varphi)}{K_s} \right) dp_{gz} + \\ & \left(\frac{\varphi S_{lq}}{K_w} \frac{\partial p_w}{\partial T} - 3\alpha_w^m \right) dT \end{aligned} \quad \text{éq 5.2.2-1}$$

$$\begin{aligned} \frac{dm_{ad}}{\rho_{ad}} = & bS_{lq} d\varepsilon_v + \left(\frac{S_{lq}\varphi M_{as}^{ol}}{\rho_{ad}K_H} \frac{\partial p_{as}}{\partial P_c} - \frac{S_{lq}^2(b-\varphi)}{K_s} + \varphi \frac{\partial S_{lq}}{\partial P_c} \right) dp_c + \\ & S_{lq} \left(\frac{\varphi M_{as}^{ol}}{\rho_{ad}K_H} \frac{\partial p_{as}}{\partial P_{gz}} + \frac{(b-\varphi)}{K_s} \right) dp_{gz} + S_{lq} \left(\frac{\varphi M_{as}^{ol}}{\rho_{ad}K_H} \frac{\partial p_{as}}{\partial T} - 3\alpha_0(b-\varphi) \right) dT \end{aligned} \quad \text{éq 5.2.2-2}$$

$$\begin{aligned} \frac{dm_{vp}}{\rho_{vp}} = & b(1-S_{lq}) d\varepsilon_v + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}(b-\varphi)}{K_s} - \frac{\varphi(1-S_{lq})\rho_{vp}}{p_{vp}\rho_{lq}} \right) dp_c + \\ & \left(\frac{(b-\varphi)(1-S_{lq})}{K_s} + \frac{\varphi(1-S_{lq})\rho_{vp}}{p_{vp}\rho_{lq}} \right) dp_{gz} + \left(-3\alpha_{vp}^m + \frac{\varphi\rho_{vp}(1-S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{vp}T} \right) dT \end{aligned} \quad \text{éq 5.2.2-3}$$

$$\frac{dm_{as}}{\rho_{as}} = b(1-S_{lq})d\varepsilon_V + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}(b-\varphi)}{K_s} + \frac{\varphi(1-S_{lq})\rho_{vp}}{P_{as}\rho_{lq}} \right) dp_c + \left(\frac{(b-\varphi)(1-S_{lq})}{K_s} + \frac{\varphi(1-S_{lq})\rho_{lq}-\rho_{vp}}{P_{as}\rho_{lq}} \right) dp_{gz} + \left(-3\alpha_{vp}^m - \frac{\varphi\rho_{vp}(1-S_{lq})(h_{vp}^m-h_{lq}^m)}{P_{as}T} \right) dT$$

éq the

5.2.2-4

partial derivatives are given in [§ Annexe 3].

5.3 Derived from the enthalpy and heat Q'

Là still, we do nothing but point out statements already provided to chapter 2:

5.3.1 Case without dissolved air

$$dh_w^m = (1-3\alpha_w T) \frac{dp_{gz} - dp_c}{\rho_w} + C_w^p dT$$

$$dh_{vp}^m = C_{vp}^p dT$$

$$dh_{as}^m = C_{as}^p dT$$

$$\delta Q' = 3\alpha_0 K_0 T d\varepsilon_V + 3\alpha_{lq}^m T dp_c - (3\alpha_{gz}^m + 3\alpha_{lq}^m) T dp_{gz} + C_\varepsilon^0 dT$$

5.3.2 Case with dissolved air

$$dh_w^m = (1-3\alpha_w T) \frac{dp_{gz} - dp_c - dp_{ad}}{\rho_w} + C_w^p dT$$

$$= \left(\frac{1-3\alpha_w T}{\rho_w} \right) \left[\left(1 - \frac{\partial p_{ad}}{\partial p_{gz}} \right) dp_{gz} - \left(1 + \frac{\partial p_{ad}}{\partial p_c} \right) dp_c \right] + \left(C_w^p - \frac{1-3\alpha_w T}{\rho_w} \frac{\partial p_{ad}}{\partial T} \right) dT$$

$$dh_{ad}^m = C_{ad}^p dT$$

$$dh_{vp}^m = C_{vp}^p dT$$

$$dh_{as}^m = C_{as}^p dT$$

$$\delta Q' = 3\alpha_0 K_0 T d\varepsilon_V + 3\alpha_{lq}^m T dp_c - (3\alpha_{gz}^m + 3\alpha_{lq}^m) T dp_{gz} + C_\varepsilon^0 dT$$

5.4 Derived from heat flux

One leaves [éq 3.2.5.1 - 1] and [éq 3.2.5.1 - 2].

While differentiating [éq 3.2.5.1 - 2] and by means of [éq 3.2.1-1], one finds:

$$d\lambda^T = (b-\varphi)\lambda_\varphi^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) d\varepsilon_V + \frac{(b-\varphi)}{K_s} \lambda_\varphi^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) dp_{gz} + \left(\lambda_\varphi^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \cdot \frac{\partial S_{lq}}{\partial P_c} - S_{lq} \frac{(b-\varphi)}{K_s} \lambda_\varphi^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \right) dp_c + \left(\lambda_\varphi^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) - (b-\varphi) \cdot 3\alpha_0 \lambda_\varphi^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \right) dT$$

That is to say finally:

$$\begin{aligned}
 dq = & -(b-\varphi) \lambda_{\varphi}^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \nabla T d \varepsilon_v \\
 & - \frac{(b-\varphi)}{K_s} \lambda_{\varphi}^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \nabla T dp_{gz} \\
 & - \left(\lambda_{\varphi}^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \cdot \frac{\partial S_{lq}}{\partial p_c} - S_{lq} \frac{(b-\varphi)}{K_s} \lambda_{\varphi}^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \right) \nabla T dp_c \\
 & - \left(\lambda_{\varphi}^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) - (b-\varphi) \cdot 3 \alpha_0 \lambda_{\varphi}^T(\varphi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) \right) \nabla T dT
 \end{aligned} \tag{éq 5.4-1}$$

5.5 Derivative of hydrous flux

It is of course necessary to set out again of the equations [éq 3.2.5.2 - 15], [éq 3.2.5.2 - 16], [éq 3.2.5.2 - 17] and [éq 3.2.5.2 - 18] which one differentiates.

5.5.1 Case without dissolved air

$$\begin{aligned}
 d \mathbf{M}_{as} = & \left(\frac{\mathbf{M}_{as}}{\rho_{as}} + \rho_{as} \lambda_{gz}^H \mathbf{F}^m \right) d \rho_{as} + \frac{\mathbf{M}_{as} - \rho_{as} C_{vp} F_{vp} \nabla C_{vp}}{\lambda_{lq}^H} d \lambda_{gz}^H \\
 & + \rho_{as} \lambda_{gz}^H \left(-d \nabla p_{gz} + d \rho_{vp} \mathbf{F}^m \right) \\
 & + \rho_{as} C_{vp} \left(\frac{\partial F_{vp}}{\partial T} dT + \frac{\partial F_{vp}}{\partial p_{gz}} p_{gz} \right) \nabla C_{vp} + \rho_{as} dC_{vp} F_{vp} \nabla C_{vp} + \rho_{as} C_{vp} F_{vp} d \nabla C_{vp}
 \end{aligned} \tag{éq 5.5.1-1}$$

$$\begin{aligned}
 d \mathbf{M}_{vp} = & \left(\frac{\mathbf{M}_{vp}}{\rho_{vp}} + \rho_{vp} \lambda_{gz}^H \mathbf{F}^m \right) d \rho_{vp} + \frac{\mathbf{M}_{vp} + \rho_{vp} (1 - C_{vp}) F_{vp} \nabla C_{vp}}{\lambda_{gz}^H} d \lambda_{gz}^H \\
 & + \rho_{vp} \lambda_{gz}^H \left(-d \nabla p_{gz} + d \rho_{as} \mathbf{F}^m \right) \\
 & - (1 - C_{vp}) \rho_{vp} \left(\frac{\partial F_{vp}}{\partial T} dT + \frac{\partial F_{vp}}{\partial p_{gz}} p_{gz} \right) \nabla C_{vp} + \rho_{vp} dC_{vp} F_{vp} \nabla C_{vp} - \rho_{vp} (1 - C_{vp}) F_{vp} d \nabla C_{vp}
 \end{aligned} \tag{éq 5.5.1-2}$$

$$\begin{aligned}
 d \mathbf{M}_w = & \left(\frac{\mathbf{M}_w}{\rho_w} + \rho_w \lambda_{lq}^H F^m \right) d \rho_w + \frac{\mathbf{M}_w}{\lambda_{lq}^H} d \lambda_{lq}^H \\
 & - \rho_w \lambda_{lq}^H \left(d \nabla p_{gz} - d \nabla p_c \right)
 \end{aligned} \tag{éq 5.5.1-3}$$

In order to completely clarify these differentials, it is necessary to know the differentials of the densities of the fluids, as well as the differentials of $C_{vp} = \frac{p_{vp}}{p_{gz}}$ and its gradient. Knowing [éq 3.2.6-4], one can then calculate the differential of the air pressure dryness:

$$dp_{as} = dp_{gz} - dp_{vp} = \frac{\rho_w - \rho_{vp}}{\rho_w} dp_{gz} + \frac{\rho_{vp}}{\rho_w} dp_c - \rho_{vp} \left(h_{vp}^m - h_w^m \right) \frac{dT}{T} \tag{éq 5.5.1-4}$$

By deriving the relation from perfect gases one a: $\frac{d \rho_{as}}{\rho_{as}} = \frac{dp_{as}}{p_{as}} - \frac{dT}{T}$ and $\frac{d \rho_{vp}}{\rho_{vp}} = \frac{dp_{vp}}{p_{vp}} - \frac{dT}{T}$, which, by means of [éq 3.2.6-4] and [éq 5.5.1-4] gives:

$$d \rho_{vp} = \frac{\rho_{vp}^2}{\rho_w p_{vp}} dp_{gz} - \frac{\rho_{vp}^2}{\rho_w p_{vp}} dp_c + \left(\frac{\rho_{vp}^2 (h_{vp}^m - h_w^m)}{T p_{vp}} - \frac{\rho_{vp}}{T} \right) dT \quad \text{éq 5.5.1-5}$$

$$d \rho_{as} = \frac{\rho_{as}}{p_{as}} \frac{\rho_w - \rho_{vp}}{\rho_w} dp_{gz} + \frac{\rho_{as}}{p_{as}} \frac{\rho_{vp}}{\rho_w} dp_c + \left(-\frac{\rho_{as} \rho_{vp} (h_{vp}^m - h_w^m)}{T p_{as}} - \frac{\rho_{as}}{T} \right) dT \quad \text{éq 5.5.1-6}$$

[éq 3.2.6-4] makes it possible to express the gradient of the steam pressure:

$$\nabla p_{vp} = \frac{\rho_{vp}}{\rho_{lq}} (\nabla p_{gz} - \nabla p_c) + \rho_{vp} (h_{vp}^m - h_{lq}^m) \frac{\nabla T}{T} \quad \text{éq 5.5.1-7}$$

While differentiating [éq 5.5.1-7] one finds:

$$d \nabla p_{vp} = \frac{\rho_{vp}}{\rho_w} (d \nabla p_{gz} - d \nabla p_c) + \left(\frac{d \rho_{vp}}{\rho_w} - \frac{\rho_{vp}}{\rho_w^2} d \rho_w \right) (\nabla p_{gz} - \nabla p_c) + \rho_{vp} \left(\frac{h_{vp}^m - h_w^m}{T} \right) d \nabla T + d \left(\rho_{vp} \left(\frac{h_{vp}^m - h_w^m}{T} \right) \right) \nabla T$$

éq 5.5.1-8

the last term of [éq 5.5.1-8] is written:

$$d \left(\rho_{vp} \left(\frac{h_{vp}^m - h_w^m}{T} \right) \right) \nabla T = \left(\frac{h_{vp}^m - h_w^m}{T} \right) \nabla T d \rho_{vp} + \frac{\rho_{vp}}{T} \nabla T (dh_{vp}^m - dh_w^m) - \rho_{vp} (h_{vp}^m - h_w^m) \nabla T \frac{dT}{T^2}$$

éq 5.5.1-9

Knowing the differentials of its gradient and steam pressure, the statements of the differentials of C_{vp} and its gradient are easy to calculate:

$$dC_{vp} = \frac{dp_{vp}}{p_{gz}} - \frac{p_{vp}}{p_{gz}^2} dp_{gz} \quad \text{who gives:} \quad \nabla C_{vp} = \frac{\nabla p_{vp}}{p_{gz}} - \frac{p_{vp}}{p_{gz}^2} \nabla p_{gz} \quad \text{and that one differentiates in:}$$

$$d \nabla C_{vp} = d \left[\frac{\nabla p_{vp}}{p_{gz}} - \frac{p_{vp}}{p_{gz}^2} \nabla p_{gz} \right] = \frac{d \nabla p_{vp}}{p_{gz}} - \frac{\nabla p_{gz}}{p_{gz}^2} dp_{vp} + \left(2 \frac{p_{vp}}{p_{gz}^3} \nabla p_{gz} - \frac{\nabla p_{vp}}{p_{gz}^2} \right) dp_{gz} - \frac{p_{vp}}{p_{gz}^2} d \nabla p_{gz}$$

dp_{vp} is given by [éq 3.2.6-4] and $d \nabla p_{vp}$ by [éq 5.5.1-8].

5.5.2 Case with dissolved air

$$\begin{aligned}
 d \mathbf{M}_{as} = & \left(\frac{\mathbf{M}_{as}}{\rho_{as}} + \rho_{as} \lambda_{gz}^H \mathbf{F}^m \right) d \rho_{as} + \frac{\mathbf{M}_{as} - \rho_{as} C_{vp} F_{vp} \nabla C_{vp}}{\lambda_{gz}^H} d \lambda_{gz}^H \\
 & + \rho_{as} \lambda_{gz}^H \left(-d \nabla p_{gz} + d \rho_{vp} \mathbf{F}^m \right) \\
 & + \rho_{as} C_{vp} \left(\frac{\partial F_{vp}}{\partial T} dT + \frac{\partial F_{vp}}{\partial p_{gz}} dp_{gz} \right) \nabla C_{vp} + \rho_{as} dC_{vp} F_{vp} \nabla C_{vp} + \rho_{as} C_{vp} F_{vp} d \nabla C_{vp}
 \end{aligned} \tag{5.5.2-1}$$

$$\begin{aligned}
 d \mathbf{M}_{vp} = & \left(\frac{\mathbf{M}_{vp}}{\rho_{vp}} + \rho_{vp} \lambda_{gz}^H \mathbf{F}^m \right) d \rho_{vp} + \frac{\mathbf{M}_{vp} + \rho_{vp} (1 - C_{vp}) F_{vp} \nabla C_{vp}}{\lambda_{gz}^H} d \lambda_{gz}^H \\
 & + \rho_{vp} \lambda_{gz}^H \left(-d \nabla p_{gz} + d \rho_{as} \mathbf{F}^m \right) \\
 & - (1 - C_{vp}) \rho_{vp} \left(\frac{\partial F_{vp}}{\partial T} dT + \frac{\partial F_{vp}}{\partial p_{gz}} dp_{gz} \right) \nabla C_{vp} + \rho_{vp} dC_{vp} F_{vp} \nabla C_{vp} - \rho_{vp} (1 - C_{vp}) F_{vp} d \nabla C_{vp}
 \end{aligned} \tag{5.5.2-2}$$

$$d \mathbf{M}_w = \left(\frac{\mathbf{M}_w}{\rho_w} + \rho_w \lambda_{lq}^H \mathbf{F}^m \right) d \rho_w + \frac{\mathbf{M}_w}{\lambda_{lq}^H} d \lambda_{lq}^H + \rho_w \lambda_{lq}^H \left(-d \nabla p_{lq} + d \rho_{ad} \mathbf{F}^m \right) \tag{5.5.2-3}$$

$$\begin{aligned}
 d \mathbf{M}_{ad} = & \left(-\lambda_{lq}^H \nabla p_{lq} + \rho_{lq} \lambda_{lq}^H \mathbf{F}^m \right) d \rho_{ad} + \rho_{ad} \left(-\lambda_{lq}^H (\nabla p_{lq} + \rho_{lq} \mathbf{F}^m) \right) d \lambda_{lq}^H \\
 & + \rho_{ad} \lambda_{lq}^H \left(-d \nabla p_{lq} + d \rho_w \mathbf{F}^m \right) \\
 & - \left(\frac{\partial F_{ad}}{\partial T} dT + \frac{\partial F_{ad}}{\partial p_c} dp_c \right) \nabla C_{ad} - F_{ad} d \nabla C_{ad}
 \end{aligned} \tag{5.5.2-4}$$

It is necessary to know the differentials of the densities of the fluids, as well as the differentials of $C_{vp} = \frac{p_{vp}}{p_{gz}}$, $C_{ad} = \rho_{ad}$ and their gradient. One first of all will calculate the differentials of the densities by means of the derivatives partial of pressures given in [§Annexe 3].

By deriving the relation from perfect gases one a: $\frac{d \rho_{as}}{\rho_{as}} = \frac{dp_{as}}{p_{as}} - \frac{dT}{T}$ and $\frac{d \rho_{vp}}{\rho_{vp}} = \frac{dp_{vp}}{p_{vp}} - \frac{dT}{T}$, which one can express in the form:

$$d \rho_{as} = \frac{\rho_{as}}{p_{as}} \left(\frac{\partial p_{as}}{\partial p_c} dp_c + \frac{\partial p_{as}}{\partial p_{gz}} dp_{gz} \right) + \left(\frac{\rho_{as}}{p_{as}} \frac{\partial p_{as}}{\partial T} - \frac{\rho_{as}}{T} \right) dT \tag{5.5.2-5}$$

$$d \rho_{vp} = \frac{\rho_{vp}}{p_{vp}} \left(\frac{\partial p_{vp}}{\partial p_c} dp_c + \frac{\partial p_{vp}}{\partial p_{gz}} dp_{gz} \right) + \left(\frac{\rho_{vp}}{p_{vp}} \frac{\partial p_{vp}}{\partial T} - \frac{\rho_{vp}}{T} \right) dT \tag{5.5.2-6}$$

By means of the relation [équ 3.2.3.1 - 1], one obtains:

$$d\rho_w = \frac{\rho_w}{K_w} \left(\frac{\partial p_w}{\partial p_c} dp_c + \frac{\partial p_w}{\partial p_{gz}} dp_{gz} \right) + \left(\frac{\rho_w}{K_w} \frac{\partial p_w}{\partial T} - 3\rho_w \alpha_w \right) dT \quad \text{éq 5.5.2-7}$$

And like $d\rho_{ad} = \frac{M_{as}^{ol}}{K_H} dp_{as}$,

$$d\rho_{ad} = \frac{M_{as}^{ol}}{K_H} \left(\frac{\partial p_{as}}{\partial p_c} dp_c + \frac{\partial p_{as}}{\partial p_{gz}} dp_{gz} + \frac{\partial p_{as}}{\partial T} dT \right) \quad \text{éq 5.5.2-8}$$

Like previously, one uses the statement:

$dC_{vp} = \frac{dp_{vp}}{p_{gz}} - \frac{p_{vp}}{p_{gz}^2} dp_{gz}$ who gives:

$$dC_{vp} = \frac{1}{p_{gz}} \left(\frac{\partial p_{vp}}{\partial p_c} dp_c + \frac{\partial p_{vp}}{\partial T} dT \right) + \left(\frac{1}{p_{gz}} \frac{\partial p_{vp}}{\partial p_{gz}} - \frac{p_{vp}}{p_{gz}^2} \right) dp_{gz} \quad \text{éq 5.5.2-9}$$

and $\nabla C_{vp} = \frac{\nabla p_{vp}}{p_{gz}} - \frac{p_{vp}}{p_{gz}^2} \nabla p_{gz}$ that one differentiates in:

$$d\nabla C_{vp} = d \left[\frac{\nabla p_{vp}}{p_{gz}} - \frac{p_{vp}}{p_{gz}^2} \nabla p_{gz} \right] = \frac{d\nabla p_{vp}}{p_{gz}} - \frac{\nabla p_{gz}}{p_{gz}^2} dp_{vp} + \left(2 \frac{p_{vp}}{p_{gz}^3} \nabla p_{gz} - \frac{\nabla p_{vp}}{p_{gz}^2} \right) dp_{gz} - \frac{p_{vp}}{p_{gz}^2} d\nabla p_{gz} \quad \text{éq 5.5.2-10}$$

with

$$\nabla p_{vp} = \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial p_{vp}}{\partial T} \nabla T \quad \text{éq 5.5.2-11}$$

and $d\nabla p_{vp}$ that one differentiates in the following way:

$$\begin{aligned} d\nabla p_{vp} &= d \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + d \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + d \frac{\partial p_{vp}}{\partial T} \nabla T + \frac{\partial p_{vp}}{\partial p_{gz}} d\nabla p_{gz} + \frac{\partial p_{vp}}{\partial p_c} d\nabla p_c + \frac{\partial p_{vp}}{\partial T} d\nabla T \\ &= \left(\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial T} \nabla T \right) dp_c \\ &+ \left(\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial T} \nabla T \right) dp_{gz} \quad \text{éq the} \\ &+ \left(\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial T} \nabla T \right) dT \\ &+ \frac{\partial p_{vp}}{\partial p_{gz}} d\nabla p_{gz} + \frac{\partial p_{vp}}{\partial p_c} d\nabla p_c + \frac{\partial p_{vp}}{\partial T} d\nabla T \end{aligned} \quad \text{5.5.2-12}$$

derivatives partial of the second order are developed in [§Annexe 4].

For the dissolved air, one proceeds with the same stages:

$$C_{ad} = \rho_{ad} = M_{ad}^{ol} \cdot \frac{P_{ad}}{RT}$$

thus:

$$dC_{ad} = M_{ad}^{ol} \cdot \left(\frac{dp_{ad}}{RT} - \frac{P_{ad}}{RT^2} dT \right) \text{ who gives:}$$

$$dC_{ad} = M_{ad}^{ol} \cdot \left[\left(\frac{1}{RT} \frac{\partial P_{ad}}{\partial p_c} \right) dp_c + \left(\frac{1}{RT} \frac{\partial P_{ad}}{\partial p_{gz}} \right) dp_{gz} + \left(\frac{\partial P_{ad}}{\partial T} - \frac{P_{ad}}{RT^2} \right) \frac{1}{p_{lq}} dT \right] \quad \text{éq 5.5.2-13}$$

$$\text{and } \nabla C_{ad} = M_{ad}^{ol} \cdot \left(\frac{\nabla P_{ad}}{RT} - \frac{P_{ad}}{RT^2} \nabla T \right) \text{ that one differentiates in:}$$

$$d \nabla C_{ad} = M_{ad}^{ol} \left[\frac{1}{RT} d \nabla P_{ad} - \frac{1 \nabla T}{RT^2} dp_{ad} + \left(2 \frac{P_{ad}}{RT^3} \nabla T - \frac{\nabla P_{ad}}{RT^2} \right) dT - \left(\frac{P_{ad}}{RT^2} \right) d \nabla T \right] \quad \text{éq 5.5.2-14}$$

with:

$$\nabla P_{ad} = \frac{\partial P_{ad}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial P_{ad}}{\partial p_c} \nabla p_c + \frac{\partial P_{ad}}{\partial T} \nabla T \quad \text{éq 5.5.2-15}$$

and $d \nabla P_{ad}$ that one differentiates in the following way:

$$\begin{aligned} &= \left(\frac{\partial}{\partial p_c} \frac{\partial P_{ad}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial p_c} \frac{\partial P_{ad}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial p_c} \frac{\partial P_{ad}}{\partial T} \nabla T \right) dp_c \\ &+ \left(\frac{\partial}{\partial p_{gz}} \frac{\partial P_{ad}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial p_{gz}} \frac{\partial P_{ad}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial p_{gz}} \frac{\partial P_{ad}}{\partial T} \nabla T \right) dp_{gz} \\ &+ \left(\frac{\partial}{\partial T} \frac{\partial P_{ad}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial T} \frac{\partial P_{ad}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial T} \frac{\partial P_{ad}}{\partial T} \nabla T \right) dT \\ &+ \frac{\partial P_{ad}}{\partial p_{gz}} d \nabla p_{gz} + \frac{\partial P_{ad}}{\partial p_c} d \nabla p_c + \frac{\partial P_{ad}}{\partial T} d \nabla T \end{aligned} \quad \text{éq the 5.5.2-16}$$

derivatives partial of the second order are developed in [§Annexe 4].

6 Bibliography

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7 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
5	C.Chavant EDF-R&D/AMA	initial Version
7.4	C.Chavant, S.Granet, EDF-R&D/AMA	
9.2	S.Granet EDF-R&D/AMA	Model of Van Genuchten
10.2	S. Meunier, EDF R & D Hydraulic	/AMA Modelization Saturated
11.2	F.Voldoire EDF-R&D/AMA	Modifications with working with the equations, some corrections here or there.

Annexe 1 Generalized stresses and local variables

stresses:

Number	Name of component Aster	Contained
1	SIXX	σ'_{xx}
2	SIYY	σ'_{yy}
3	SIZZ	σ'_{zz}
4	SIXY	σ'_{xy}
5	SIXZ	σ'_{xz}
6	SIYZ	σ'_{yz}
7	SIP	σ_p
8	M11	m_w
9	FH11X	M_{w_x}
10	FH11Y	M_{w_y}
11	FH11Z	M_{w_z}
12	ENT11	h_w^m
13	M12	m_{vp}
14	FH12X	M_{vp_x}
15	FH12Y	M_{vp_y}
16	FH12Z	M_{vp_z}
17	ENT12	h_{vp}^m
18	M21	m_{as}
19	FH21X	M_{as_x}
20	FH21Y	M_{as_y}
21	FH21Z	M_{as_z}
22	ENT21	h_{as}^m
18	M22	m_{ad}
19	FH22X	M_{ad_x}
20	FH22Y	M_{ad_y}
21	FH22Z	M_{ad_z}
22	ENT22	h_{ad}^m
23	QPRIM	Q'
24	FHTX	q_x
25	FHTY	q_y

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FHTZ

q_z

In the case without mechanics, and for constitutive laws (LIQU_VAPE_GAZ, LIQU_VAPE, LIQU_AD_GAZ_VAPE and LIQU_AD_GAZ) the local variables are:

Number	Name of component Code_Aster	Contained
1	V1	$\rho_{lq} - \rho_{lq}^0$
2	V2	$\varphi - \varphi^0$
3	V3	$p_{vp} - p_{vp}^0$
4	V4	S_{lq}

In the case without mechanics, and for constitutive laws (LIQU_GAZ, LIQU_GAZ_ATM,) the local variables are:

Number	Name of component Code_Aster	Contained
1	V1	$\rho_{lq} - \rho_{lq}^0$
2	V2	$\varphi - \varphi^0$
3	V3	S_{lq}

In the case without mechanics, and for constitutive laws (LIQU_SATU,) the local variables are:

Number	Name of component Code_Aster	Contained
1	V1	$\rho_{lq} - \rho_{lq}^0$
2	V2	$\varphi - \varphi^0$

In the case with mechanics the first numbers will be those corresponding to the mechanics (v1 in the elastic case, v1 and following for plastic models). The number of the local variables above will have to then be incremented of as much.

Annexe 2 Material characteristics

One gives here the correspondence between the vocabulary of the Aster commands and the notations used in the present note for the various quantities characteristic of the materials.

A2.1 Key word factor THM_LIQU

◆	RHO	ρ_{lq}^0
◇	UN_SUR_K	$\frac{1}{K_{lq}}$
◇	ALPHA	α_{lq}
◇	CP	C_{lq}^p
◇	VISC	$\mu_{lq}(T)$
◇	D_VISC_TEMP	$\frac{\partial \mu_{lq}}{\partial T}(T)$

A2.2 Key word factor THM_GAZ

◇	MASS_MOL	M_{as}^{ol}
◇	CP	C_{lq}^P
◇	VISC	$\mu_{as}(T)$
◇	D_VISC_TEMP	$\frac{\partial \mu_{as}}{\partial T}(T)$

A2.3 Key word factor THM_VAPE_GAZ

◇	MASS_MOL	M_{VP}^{ol}
◇	CP	C_{vp}^P
◇	VISC	$\mu_{vp}(T)$
◇	D_VISC_TEMP	$\frac{\partial \mu_{vp}}{\partial T}(T)$

A2.4 Key word factor THM_AIR_DISS

◇	CP	C_{ad}^P
◇	COEF_HENRY	K_H

A2.5 Key word factor THM_INIT

◆	TEMP	$^{init} T$
◆	PRE1	$^{init} P_1$
◆	PRE2	$^{init} P_2$
◆	PORO	Φ^0
◆	PRES_VAPE	P_{vp}^0

One recalls that, according to the modelization, the two pressures P_1 and P_2 represent:

	LIQU_SATU	LIQU_VAPE	LIQU_GAZ_ATM	GAZ	LIQU_VAPE_GAZ
P_1	p_w	p_w	$p_c = -p_w$	p_{gz}	$p_c = p_{gz} - p_w$
P_2					p_{gz}

	LIQU_GAZ	LIQU_AD_GAZ_VAPE	LIQU_AD_GAZ
P_1	$p_c = p_{gz} - p_w$	$p_c = p_{gz} - p_w - p_{ad}$	$p_c = p_{gz} - p_w - p_{ad}$
P_2	p_{gz}	p_{gz}	p_{gz}

A2.6 Key word factor THM_DIFFU

◆	R_GAZ	R
◇	RHO	r_0
◇	CP	C_{σ}^S
◇	BIOT_COEF	b

◇	SATU_PRES	$S_{lq}(p_c)$
◇	D_SATU_PRES	$\frac{\partial S_{lq}}{\partial p_c}(p_c)$
◇	PESA_X	\mathbf{F}_x^m
◇	PESA_Y	\mathbf{F}_y^m
◇	PESA_Z	\mathbf{F}_z^m
◇	PERM_IN	$K^{int}(\varphi)$
◇	PERM_LIQU	$K_{lq}^{rel}(S_{lq})$
◇	D_PERM_LIQU_SATU	$\frac{\partial K_{lq}^{rel}}{\partial S_{lq}}(S_{lq})$
◇	PERM_GAZ	$k_{gz}^{rel}(S_{lq}, p_{gz})$
◇	D_PERM_SATU_GAZ	$\frac{\partial k_{gz}^{rel}}{\partial S_{lq}}(S_{lq}, p_{gz})$
◇	D_PERM_PRES_GAZ	$\frac{\partial k_{gz}^{rel}}{\partial p_{gz}}(S_{lq}, p_{gz})$
◇	FICKV_T	$f_{vp}^T(T)$
◇	FICKV_S	$f_{vp}^S(S)$
◇	FICKV_PG	$f_{vp}^{gz}(P_g)$
◇	FICKV_PV	$f_{vp}^{vp}(P_{vp})$
◇	D_FV_T	$\frac{\partial f_{vp}^T}{\partial T}(T)$
◇	D_FV_PG	$\frac{\partial f_{vp}^{gz}}{\partial P_{gz}}(P_{gz})$
◇	FICKA_T	$f_{ad}^T(T)$
◇	FICKA_S	$f_{ad}^S(S)$
◇	FICKA_PA	$f_{ad}^{ad}(P_{ad})$
◇	FICKA_PL	$f_{ad}^{lq}(P_{lq})$
◇	D_FA_T	$\frac{\partial f_{vp}^T}{\partial T}(T)$
◇	LAMB_T	$\lambda_T^T(T)$
◇	DLAMB_T	$\frac{\partial \lambda_T^T}{\partial T}(T)$
◇	LAMB_PHI	$\lambda_\phi^T(\phi)$
◇	DLAMBPHI	$\frac{\partial \lambda_\phi^T}{\partial \phi}(\phi)$
◇	LAMB_S	$\lambda_S^T(S)$
◇	DLAMBS	$\frac{\partial \lambda_S^T}{\partial S}(S)$
◇	LAMB_CT	λ_{CT}^T

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Note:

For the modelizations utilizing the thermal, and for the computation of the homogenized specific heat, one uses the relation: $C_{\sigma}^0 = (1-\varphi)\rho_s C_{\sigma}^s + \rho_{lq} S_{lq} \varphi C_{lq}^p + (1-S_{lq})\varphi(\rho_{vp} C_{vp}^p + \rho_{as} C_{as}^p)$. In this formula, one confuses ρ_s with his initial value ρ_s^0 whose value is read under the key word *RHO* of the key word factor *ELAS*.

Annexe 3 Derived from the pressures according to the generalized strains

One details here the computation of derivatives of pressure according to the generalized strains. It is pointed out that the equation [éq 3.2.6.3] is $\frac{dp_{vp}}{\rho_{vp}} = \frac{dp_w}{\rho_w} + L \frac{dT}{T}$ with $L = h_{vp}^m - h_w^m$. Moreover

$dp_{ad} = dp_{lq} - dp_w = \frac{R}{K_H} p_{as} dT + \frac{RT}{K_H} dp_{as}$ and $dp_{as} = dp_{gz} - dp_{vp}$. By combining these equations one obtains:

$$\begin{cases} dp_{vp} \left[\frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}} \right] = (-L\rho_w + p_{ad}) \frac{dT}{T} + \left(\frac{RT}{K_H} - 1 \right) dp_{gz} + dp_c \\ dp_w \left[\frac{\rho_{vp} RT}{\rho_w K_H} - 1 \right] = \left(-LR \frac{\rho_{vp}}{K_H} + \frac{p_{ad}}{T} \right) dT + \left(\frac{RT}{K_H} - 1 \right) dp_{gz} + dp_c \end{cases}$$

One can thus write derivatives partial of water and the vapor according to the generalized strains:

$$\begin{aligned} \frac{\partial p_w}{\partial T} &= \frac{-LR \frac{\rho_{vp}}{K_H} + \frac{p_{ad}}{T}}{\frac{\rho_{vp} RT}{\rho_w K_H} - 1}; & \frac{\partial p_w}{\partial p_{gz}} &= \frac{\frac{RT}{K_H} - 1}{\frac{\rho_{vp} RT}{\rho_w K_H} - 1}; & \frac{\partial p_w}{\partial p_c} &= \frac{1}{\frac{\rho_{vp} RT}{\rho_w K_H} - 1} \\ \frac{\partial p_{vp}}{\partial T} &= \frac{(-L\rho_w + p_{ad})}{\frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}}} \cdot \frac{1}{T}; & \frac{\partial p_{vp}}{\partial p_{gz}} &= \frac{\frac{RT}{K_H} - 1}{\frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}}}; & \frac{\partial p_{vp}}{\partial p_c} &= \frac{1}{\frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}}} \end{aligned}$$

The relations $dp_{as} = dp_{gz} - dp_{vp}$ and $dp_{ad} = dp_{gz} - dp_c - dp_w$ make it possible to derive all the pressures, since one will have:

$$\frac{\partial p_{as}}{\partial T} = -\frac{\partial p_{vp}}{\partial T}; \quad \frac{\partial p_{as}}{\partial p_{gz}} = 1 - \frac{\partial p_{vp}}{\partial p_{gz}}; \quad \frac{\partial p_{as}}{\partial p_c} = -\frac{\partial p_{vp}}{\partial p_c}$$

and

$$\frac{\partial p_{ad}}{\partial T} = -\frac{\partial p_w}{\partial T}; \quad \frac{\partial p_{ad}}{\partial p_{gz}} = 1 - \frac{\partial p_w}{\partial p_{gz}}; \quad \frac{\partial p_{ad}}{\partial p_c} = -1 - \frac{\partial p_w}{\partial p_c}$$

Annexe 4 Second derivative of air and steam pressures dissolved according to the generalized strains

One calculates here derivatives partial of the second order of the steam pressure necessary to the section [5.5.2]. One will note thereafter:

$$A1 = \frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}} \quad \text{and} \quad A2 = \frac{\rho_w}{\rho_{vp}} \left(\frac{RT}{K_H} - 1 \right)$$

$$A3 = \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial T} - \frac{1}{T} - \frac{1}{K_w} \frac{\partial p_w}{\partial T} - 3\alpha_w$$

$$A4 = -\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial T} + \frac{1}{T} + \frac{1}{K_w} \frac{\partial p_w}{\partial T} - 3\alpha_w$$

Second derivative of the steam pressure:

$$\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_{gz}} = \frac{A2}{AI^2} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_c} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_{gz}} = \frac{A2}{AI^2} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_{gz}} = \frac{R}{K_H AI} - \frac{1}{AI^2} \left(\frac{RT}{K_H} - 1 \right) \left(\frac{R}{K_H} - \frac{\rho_w}{\rho_{vp}} A4 \right)$$

$$\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_c} = -\frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_c} \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_c} = -\frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_c} = -\frac{1}{AI^2} \left(\frac{R}{K_H} - \frac{\rho_w}{\rho_{vp}} A4 \right)$$

$$\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial T} = -\frac{1}{T} \frac{1}{AI^2} \left(AI \left(1 - \frac{\partial p_w}{\partial p_c} \left(1 + L \frac{\rho_w}{K_w} \right) \right) + (p_{ad} - L\rho_w) \frac{\rho_w}{\rho_{vp}} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_c} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} \right) \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial T} = -\frac{1}{T} \frac{1}{AI^2} \left(AI \left(1 - \frac{\partial p_w}{\partial p_{gz}} \left(1 + L \frac{\rho_w}{K_w} \right) \right) + (p_{ad} - L\rho_w) \frac{\rho_w}{\rho_{vp}} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} \right) \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial T} = \frac{1}{T \cdot AI} \left(\frac{\partial p_{ad}}{\partial T} - L \left(\frac{\rho_w}{K_w} \frac{\partial p_w}{\partial T} - 3\alpha_w \rho_w \right) \right) - \frac{1}{T^2 \cdot AI^2} \left(\frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}} + T \left(\frac{R}{K_H} - \frac{\rho_w}{\rho_{vp}} A4 \right) \right) (p_{ad} - L\rho_w)$$

Second derivative of the dissolved air pressure:

$$\frac{\partial}{\partial p_c} \frac{\partial p_{ad}}{\partial p_{gz}} = \frac{RT}{K_H} \frac{A2}{AI^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_c} \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{ad}}{\partial p_{gz}} = \frac{RT}{K_H} \frac{A2}{AI^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{ad}}{\partial p_{gz}} = -R_{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI} + \left(\frac{\rho_w}{\rho_{vp}} \right)^2 \frac{R}{K_H} \frac{A2}{AI^2} (1 + A3 \cdot T)$$

$$\frac{\partial}{\partial p_c} \frac{\partial p_{ad}}{\partial p_c} = \frac{RT}{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_c} \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{ad}}{\partial p_c} = \frac{RT}{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{ad}}{\partial p_c} = \frac{R}{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} (1 + A3 \cdot T)$$

$$\frac{\partial}{\partial p_c} \frac{\partial p_{ad}}{\partial T} = \frac{1}{AI} \frac{\rho_w}{\rho_{vp}} \left(\frac{LR}{K_H} \frac{\rho_{vp}}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} - \frac{1}{T} \frac{\partial p_{ad}}{\partial p_c} \right) - \frac{RT}{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{LR}{K_H} \rho_{vp} - \frac{p_{ad}}{T} \right) \cdot A3$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{ad}}{\partial T} = \frac{1}{AI} \frac{\rho_w}{\rho_{vp}} \left(\frac{LR}{K_H} \frac{\rho_{vp}}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} - \frac{1}{T} \frac{\partial p_{ad}}{\partial p_{gz}} \right) - \frac{RT}{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{LR}{K_H} \rho_{vp} - \frac{p_{ad}}{T} \right) \cdot A3$$

$$\frac{\partial}{\partial T} \frac{\partial p_{ad}}{\partial T} = \frac{1}{AI} \frac{\rho_w}{\rho_{vp}} \left(\frac{LR}{K_H} \rho_{vp} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial T} - \frac{1}{T} \right) + \frac{p_{ad}}{T^2} - \frac{1}{T} \frac{\partial p_{ad}}{\partial T} \right) - \frac{RT}{K_H} \frac{\rho_w}{\rho_{vp}} \frac{1}{AI^2} \left(\frac{LR}{K_H} \rho_{vp} - \frac{p_{ad}}{T} \right) \cdot \left(A3 + \frac{1}{T} \right)$$

Annexe 5 Equivalence with formulations ANDRA

In order to be able to fit in the platform ALLIANCE, it is necessary to be coherent with the formulations posed by the ANDRA in the document [bib11]. We propose here an equivalence between the notations which would be dissimilar. These differences relate to only the writing of:

- The equation of energy
- the model of Henry
- the diffusion in the fluid
- the diffusion in gas

Notices concerning the enthalpi:

It is required to have coherence between the two models which the user of Code_Aster takes:
 $h_{lq}^{m_0} = 0$ and $h_{vp}^{m_0} = L_0$.

A5.1 Equation of energy

the table above points out the two formulations:

Notations Code_Aster	Notations ANDRA
h_{lq}^m	$= \frac{\phi_w}{\rho_w S_w n}$
h_{vp}^m	$= \frac{\phi_v}{\rho_v (1 - S_w) n}$
h_{as}^m	$= \frac{\phi_{as}}{\rho_{as} (1 - S_w) n}$
\mathbf{M}_{lq}	$= \rho_w f_w$
\mathbf{M}_{as}	$= \rho_{as} f_{as}$
\mathbf{M}_{vp}	$= \rho_v f_v$

By rewriting the equation of the energy of Code_Aster with these notations, one finds:

$$\begin{aligned} & \frac{d\phi}{dt} + Div \left(\phi_w \frac{f_w}{S_w n} + \phi_{as} \frac{f_{as}}{(1 - S_w) n} + \phi_v \frac{f_v}{(1 - S_w) n} \right) + Div(\mathbf{q}) - (T - T^0) \frac{d}{dt} [(1 - n) \rho_s C_s] \\ & + 3 \alpha_0 K_0 T \frac{d\varepsilon_v}{dt} + 3 \alpha_{lq}^m T \frac{dp_c}{dt} - 3 (\alpha_{lq}^m + \alpha_{gz}^m) T \frac{dp_{gz}}{dt} - 9 TK_0 \alpha_0^3 \frac{dT}{dt} \\ & = (\rho_w f_w + \rho_v f_v + \rho_{as} f_{as}) \mathbf{g} + \Theta \end{aligned}$$

The first line being that of the ANDRA and the others being a priori negligible.

A5.2 Model of Henry

In the formulation of the ANDRA, the formulation of Henry is given by $\omega_l^a = \frac{P_{as}}{H} \frac{M_{as}^{ol}}{M_w} \rho_w$ with the concentration of air in water that have can bring back it to a density such as $\omega_l^a = \rho_{ad}$. H express yourself in Pa.

In the formulation of *Code_Aster*, one recalls that the model of Henry is expressed in the form:

$$C_{ad}^{ol} = \frac{\rho_{ad}}{M_{ad}^{ol}} \quad \text{with} \quad C_{ad}^{ol} = \frac{P_{as}}{K_H} . \quad K_H \quad \text{express yourself in} \quad Pa \cdot m^3 \cdot mol^{-1} .$$

There is thus equivalence:

$$K_H = H \frac{M_w}{\rho_w}$$

A5.3 Diffusion of the vapor in the air

In formulation ANDRA the steam flux in the air according to the steam concentration in the air or of the relative humidity is noted:

$$f_{Diff_v} = -D_v \cdot \nabla \omega_g^e$$

with the concentration defined as the molar ratio in gas: $\omega_g^e = \frac{n_v}{n_g}$.

In *Code_Aster*, this same flux is written: $f_{Diff_v} = F_{vp} \nabla C_{vp}$ with the coefficient of Fick vapor

$F_{vp} = \frac{D_{vp}}{C_{vp}(1-C_{vp})}$ and D_{vp} the coefficient of diffusion of Fick of the gas mixture. C_{vp} is defined

like the ratio of the pressures such as: $C_{vp} = \frac{P_{vp}}{P_{gz}}$.

The model of perfect gases makes it possible to write that $C_{vp} = \omega_g^e$ thus $\nabla \omega_g^e = \nabla C_{vp}$ and $f_{Diff_v} = D_v \cdot \nabla C_{vp}$.

Thus *Code_Aster/ANDRA equivalence* is written simply:

$$F_{vp} = D_v .$$

A5.4 Diffusion of the air dissolved in water

In formulation ANDRA the flux of air dissolved in water is expressed

$$f_{a_{ds}} = D_a \cdot \nabla \omega_l^a$$

with $\omega_l^a = \frac{\rho_{ad}}{M_{ad}^{ol}}$.

In *Code_Aster*, this same flux is written: $f_{a_{ds}} = F_{ad} \nabla C_{ad}$ with the coefficient of air-dissolved Fick

$F_{ad} = \frac{D_{ad}}{C_{ad}(1-C_{ad})}$ and D_{ad} the coefficient of diffusion of Fick of the liquid mixture. C_{ad} is defined

such as: $C_{ad} = w_l^a$. Thus:

$$F_{ad} = D_a .$$