Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 1/62
Clé : R7.01.11 Révision :
3731397193c7

Models of behavior THHM

Summary:

This note introduces a family of laws of behavior `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 deformations. The relations presented here can be coupled with any law of mechanical behavior, subject making the assumption known as of the effective constraints of Bishop and that the mechanical law of behavior defines constant rubber bands (useful for the coupled terms). The purely mechanical part of the laws is not presented.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 2/62
Clé : R7.01.11 Révision : 3731397193c7

Contents

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 3/62
Clé : R7.01.11 Révision :
3731397193c7

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 4/62
Clé : R7.01.11   Révision   :
3731397193c7

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 *Page : 5/62*
Clé : R7.01.11 *Révision   :*
3731397193c7

1   Introduction

We introduce here a family of laws of behavior 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 deformations. The relations presented here can be coupled with any law of mechanical behavior, subject making the assumption known as of the effective constraints of Bishop and that the mechanical law of behavior defines constant rubber bands (useful for the coupled terms). For this reason, the purely mechanical part of the laws is not presented here.

Modelings selected are based on the presentation of the porous environments elaborate in particular by O. Coussy [1]. The relations of behavior are obtained starting from thermodynamic considerations and with arguments of homogenisation which we do not present here, and who are entirely described in the document of P. Charles [2]. In the same way the general writing of the conservation and equilibrium equations is not detailed, and one returns the reader to the documents [R5.03.01] [3] and [R7.01.10] [4], which contain definitions useful for the comprehension of this document.

The mechanics of the porous environments gathers a very exhaustive collection of physical phenomena concerning to the solids and the fluids. It makes the assumption of a coupling between the mechanical evolutions of the solids and the fluids, seen like continuous mediums, 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 mechanical, hydraulic and thermal behavior. 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 the order STAT_NON_LINE, according to the following nomenclature:

Modeling	Phenomena taken into account
KIT_H	Hydraulics with an unknown pressure
KIT_HM	Mechanics, hydraulics with an unknown pressure
KIT_HHM	Mechanics, hydraulics with two unknown pressures
KIT_THH	Thermics, hydraulics with two unknown pressures
KIT_THM	Thermics, mechanics, hydraulics with an unknown pressure
KIT_THHM	Thermics, mechanics, hydraulics with two unknown pressures

The document present describes the laws for the case more the general known as THHM. The simpler cases are obtained starting from the case general by simply cancelling the quantity absent.

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 6/62
Clé : R7.01.11 Révision :
3731397193c7

2 Presentation of the problem: Assumptions, Notations

In this chapter, one mainly endeavours to show the porous environment and his 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 (liquid 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 liquid and the gas, the interfaces solid fluid/being neglected.

2.2 Notations

We suppose that the pores of the 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. Sizes X associated with the phase j ($j=1,2$) fluid i will be noted: X_{ij} . When there are two components besides the solid, they are a liquid (typically water) and a gas (typically dry air), knowing that the liquid 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 the solid, that can be a liquid 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 the current moment is noted Ω , its border $\partial\Omega$. It is noted $\Omega_0, \partial\Omega_0$ at the initial moment.

The medium is defined by:

- parameters (vector position x , time t),
- variables (displacements, pressures, temperature),
- intrinsic sizes (forced and mass deformations, contributions, heat, enthali, flows hydraulic, thermics…).

The general assumptions carried out are the following ones:

- assumption of small displacements,
- reversible thermodynamic evolutions (not necessarily for mechanics),
- behavior isotropic, isotropic transverse (3D), orthotropic (2D),
- the gases are perfect gases,
- ideal mixture of perfect gases (total pressure = nap of the partial pressures),
- thermodynamic balance between the phases of the same component.

The various notations are clarified hereafter.

2.2.1 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:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 7/62
Clé : R7.01.11   Révision   :
3731397193c7

- geometrical variables,
- variables of thermodynamic state.

2.2.1.1 Geometrical variables

In all that follows, one adopts a Lagrangian representation compared to the skeleton (within the meaning of [1]) and coordinates $\mathbf{x} = \mathbf{x}_s(t)$ are those of a material point attached to the skeleton. All the space operators of derivation are defined compared to these coordinates.

Displacements of the skeleton 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 for the dissolved air,
  as for the dry air,
  vp for 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, thermodynamic balance between its phases imposes a relation between the steam pressure and the pressure of the liquid of this component. Finally, there is only one independent pressure per component, just as there is only one conservation equation of the mass. The number of independent pressures is thus equal to the number of independent components. The choice of these pressures is free (combinations of the pressures of the components) provided that the pressures chosen, associated with the temperature, form a system of independent variables.

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:

- total 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 modeling 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 steam pressure saturating at the same temperature) physically accessible. Modeling 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) HR are connected by the law of Kelvin.

For the typical case of the behavior known as 'LIQU_GAZ_ATM'one makes L' assumption known as of Richards: the pores are not saturated by the liquid, but the pressure of gas is supposed to be constant and the only variable of pressure is the pressure of liquid.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 8/62
Clé : R7.01.11   Révision   :
3731397193c7

2.2.1.3 Descriptive fields of the medium

The principal unknown factors, which are also the nodal unknown factors (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 modelings KIT_HM, KIT_HHM, KIT_THM, KIT_THHM,
- the temperature $T(\mathbf{x},t)$ for modelings KIT_THH, KIT_THM, KIT_THHM,
- two pressures $p_1(\mathbf{x},t), p_2(\mathbf{x},t)$ (which is $p_c(\mathbf{x},t)$, $p_{gz}(\mathbf{x},t)$ in the case studied) for modelings 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 liquid or a gas) for modelings KIT_H, KIT_HM, KIT_THM.

2.2.2 Derivative particulate

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 skeleton.

That is to say a an unspecified field on Ω, that is to say $\mathbf{x}_s(t)$ the punctual coordinate attached to the skeleton that we follow in his movement and is $\mathbf{x}_{fl}(t)$ the punctual coordinate attached to the fluid. One notes $\dot{a} = \dfrac{d^S a}{dt}$ the temporal derivative in the movement of the skeleton:

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

$\dot{a}$ is called particulate and often noted derivative $\dfrac{da}{dt}$. We prefer to use a notation which recalls that the configuration used to locate a particle is that of the skeleton by report to which a particle of fluid has a relative speed. For a particle of fluid the location $x_s(t)$ is unspecified, i.e. that the particle of fluid which occupies the position $\mathbf{x}_s(t)$ at the moment t is not the same one as that which occupies the position $\Omega^0(1+\varepsilon_V)(1-\varphi) = \Omega^0(1-\varphi^0)(1+\varepsilon_{Vs})$ at another moment t'.

2.2.3 Sizes

The equilibrium equations are:

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

The writing of these equations is given in the document [R7.01.10] [4], which defines also what we call in a general way a law of behavior THM and gives the definitions of the constraints and generalized deformations. This document uses these definitions. The equilibrium equations utilize directly the generalized constraints.
The generalized constraints are connected to the deformations generalized by the laws of behavior. The generalized deformations are calculated directly starting from the variables of state and their temporal space gradients.
The laws of behaviors can use additional quantities, often arranged in the internal variables. We gather here under the term of size at the same time the constraints, the deformations and of the additional sizes.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 9/62
Clé : R7.01.11 Révision :
3731397193c7

2.2.3.1   Sizes characteristic of the heterogeneous medium

- Porosity eulérienne: φ .
  If one notes $\Omega_{(\varphi)}$ the part of 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 porosity eulérienne.

- Saturation in liquid: S_{lq}
  If one notes Ω_{lq} the total volume occupied by the liquid, 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.

- Densities eulériennes of water ρ_w , dissolved air ρ_{ad} , dry air ρ_{as} , vapor ρ_{vp} , gas ρ_{gz} .
  If one notes γ_w (resp γ_{ad} , γ_{as} , γ_{vp}) water masses (resp of dissolved air, dry air and vapor) contents in a volume of Ω skeleton in the current configuration, one has by definition:

$$\gamma_w = \int_\Omega \rho_w S_{lq} \varphi \, d\Omega \quad \gamma_{ad} = \int_\Omega \rho_{ad} S_{lq} \varphi \, d\Omega$$
$$\gamma_{as} = \int_\Omega \rho_{as} (1 - S_{lq}) \varphi \, d\Omega \quad \gamma_{vp} = \int_\Omega \rho_{vp} (1 - S_{lq}) \varphi \, d\Omega$$

  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 initial values of the densities.

- Lagrangian homogenized density: r .
  At the moment 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 deformations $\boldsymbol{\varepsilon}(\mathbf{u})(\mathbf{x},t) = \frac{1}{2}(\nabla \mathbf{u} + {}^T\nabla \mathbf{u})$.

  One will note $\epsilon_V = tr(\boldsymbol{\varepsilon})$.
- The tensor of the constraints which are exerted on the porous environment: $\boldsymbol{\sigma}$.
  This tensor breaks up into a tensor of the effective constraints plus a tensor of constraints of pressure, $\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \boldsymbol{\sigma}_p$ and $\boldsymbol{\sigma}_p$ are components of the constraints generalized. This cutting is finally rather arbitrary, but corresponds all the same to an assumption rather commonly allowed, at least for the mediums saturated with liquid.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 10/62
Clé : R7.01.11   Révision   :
3731397193c7

2.2.3.3 Hydraulic sizes

- Mass contributions in components $m_w, m_{ad}, m_{vp}, m_{as}$ (unit: kilogramme per cubic meter).
  They represent the mass of fluid brought between the initial and current moments. They belong to the generalized constraints.

- Hydraulic flows $\mathbf{M}_w, \mathbf{M}_{ad}, \mathbf{M}_{vp}, \mathbf{M}_{as}$ (unit: kilogramme/second/square meter).
  One could not give very well no more precise definition of the contributions of mass and flows, considering that their definition is summarized to check the equilibrium equations hydraulic:

$$\begin{cases} \dot{m}_w + \dot{m}_{vp} + Div\left(\mathbf{M}_w + \mathbf{M}_{vp}\right) = 0 \\ \dot{m}_{as} + \dot{m}_{ad} + Div\left(\mathbf{M}_{as} + \mathbf{M}_{ad}\right) = 0 \end{cases}$$

éq 2.2.3.3 - 1

We nevertheless will specify the physical direction as of these sizes, knowing that what we write now is already a law of behavior.
Speeds of the components are measured in a fixed reference frame in space and time.

One notes $\mathbf{v}_w$ the speed 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 $\mathbf{v}_S = \dfrac{d\,\mathbf{u}}{dt}$ that of the skeleton.
The mass contributions are defined by:

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

éq 2.2.3.3 - 2

Mass flows are defined by:

$$\begin{aligned} \mathbf{M}_w &= \rho_w\varphi\,S_l\left(\mathbf{v}_w - \mathbf{v}_s\right) \\ \mathbf{M}_{ad} &= \rho_{ad}\varphi\,S_l\left(\mathbf{v}_{ad} - \mathbf{v}_s\right) \\ \mathbf{M}_{as} &= \rho_{as}\varphi\left(1-S_l\right)\left(\mathbf{v}_{as} - \mathbf{v}_s\right) \\ \mathbf{M}_{vp} &= \rho_{vp}\varphi\left(1-S_l\right)\left(\mathbf{v}_{vp} - \mathbf{v}_s\right) \end{aligned}$$

éq 2.2.3.3 - 3

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

$$r = r_0 + m_w + m_{ad} + m_{vp} + m_{as}$$

éq 2.2.3.3 - 4

where r_0 indicate the density homogenized at the initial moment.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 11/62
Clé : R7.01.11 Révision :
3731397193c7

Other intermediate hydraulic sizes are introduced:

- concentration of the vapor in gas: $C_{vp} = \dfrac{p_{vp}}{p_{gz}}$,

- gas flow: $\dfrac{\mathbf{M}_{gz}}{\rho_{gz}} = (1 - C_{vp}) \dfrac{\mathbf{M}_{as}}{\rho_{as}} + C_{vp} \dfrac{\mathbf{M}_{vp}}{\rho_{vp}}$. This equation specifies that the speed of gas is obtained by making an average (balanced sum) speeds 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 enthali of the components h_{ij}^m ($h_w^m, h_{ad}^m, h_{vp}^m, h_{as}^m$) (unit: Joule/Kelvin/kilogramme),
- heat flow: $\mathbf{q}$ (unit: $J/s/m^2$).

All these sizes belong to the constraints generalized within the meaning of the document [R7.01.10] [4].

2.2.4 External data

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

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] [4].

3.1.1 Mechanical balance

While noting σ the tensor of the total mechanical constraints and r the homogenized density of the medium, mechanical balance is written:

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

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

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 12/62
Clé : R7.01.11   Révision :
3731397193c7

3.1.2 Conservation of the fluid masses

For the fluid the derivative $\dot{a} = \dfrac{d^s a}{dt}$ is in fact a derivative eulérienne 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 unknown factors. The conservation equations of the fluid masses are written then:

$$\begin{cases} \dot{m}_w + \dot{m}_{vp} + Div(M_w + M_{vp}) = 0 \\ \dot{m}_{as} + \dot{m}_{ad} + Div(M_{as} + M_{ad}) = 0 \end{cases}$$

éq 3.1.2-1

3.1.3 Conservation of energy: thermal equation

$$h_w^m \dot{m}_w + h_{ad}^m \dot{m}_{ad} + h_{vp}^m \dot{m}_{vp} + h_{as}^m \dot{m}_{as} + \dot{Q}' + Div\left(h_w^m \mathbf{M}_w + h_{ad}^m \mathbf{M}_{ad} + h_{vp}^m \mathbf{M}_{vp} + h_{as}^m \mathbf{M}_{as}\right) + Div(\mathbf{q}) =$$
$$\left(\mathbf{M}_w + \mathbf{M}_{ad} + \mathbf{M}_{vp} + \mathbf{M}_{as}\right) F^m + \Theta$$

éq 3.1.3-1

3.2 Equations of behavior

3.2.1 Evolution of porosity

3.2.1.1 Isotropic case general

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

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 module of compressibility of the solid matter constituents. If K_0 indicate the module of compressibility "drained" of the porous environment, one has the relation:

$$b = 1 - \frac{K_0}{K_s}$$

éq 3.2.1-2

Notice :

Expression 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 porosity eulérienne 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:

$$\Phi = (1 + \varepsilon_V)\varphi$$

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 variation of volume:

$$d\Phi = b . d\varepsilon_V$$

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 modelings THM), one obtains $d\varphi = (b - \varphi) d\varepsilon_V$, which corresponds well to [éq 3.2.1-1] for the examined case.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 13/62
Clé : R7.01.11   Révision   :
3731397193c7

3.2.1.2 Transverse isotropic case

$$d\,\varphi = \boldsymbol{B} : \boldsymbol{d}\,\varepsilon - \varphi\,d\,\varepsilon_V - 3\,\alpha_\varphi\,dT + \frac{dp_{gz} - S_{lq}\,dp_c}{M_\varphi}$$

éq 3.2.1-5

In this equation, one sees appearing the tensor of Biot $\boldsymbol{B}$, the module of Biot of the solid matrix $\frac{1}{M_\varphi}$ and α_φ the differential dilation coefficient.

The expression of the differential dilation coefficient is given by the relation:

$$\alpha_\varphi = \frac{(\boldsymbol{B} - \varphi\,\boldsymbol{\delta}) : \boldsymbol{\alpha_0}}{3}$$

éq 3.2.1-6

- δ the matrix identity,
- $\boldsymbol{B} = (b_L(\boldsymbol{e_L} \otimes \boldsymbol{e_L} + \boldsymbol{e_T} \otimes \boldsymbol{e_T}) + b_N(\boldsymbol{e_N} \otimes \boldsymbol{e_N}))$ the tensor of Biot function of the average coefficients of Biot b_L and b_N according to the directions NR and L of the local reference mark of orthotropism (L, T, NR). In the isotropic case $b_L = b_N = b$,
- $\boldsymbol{\alpha_0} = (\alpha_L(\boldsymbol{e_L} \otimes \boldsymbol{e_L} + \boldsymbol{e_T} \otimes \boldsymbol{e_T}) + \alpha_N(\boldsymbol{e_N} \otimes \boldsymbol{e_N}))$ the thermal tensor of dilation function of α_N and α_L average coefficients of dilation of the porous environments and the solid matter constituents according to the directions NR and L of the local reference mark of orthotropism (L, T, NR). In the isotropic case $\alpha_L = \alpha_N = \alpha_0$.

Note:

In the isotropic case the expression of the differential dilation coefficient is given by:

$$\alpha_\varphi = (b - \varphi)\alpha_0$$

The expression of the module of Biot of the solid matrix is given by the following relation ([11] and [13]) :

$$\frac{1}{M_\varphi} = (\boldsymbol{B} - \varphi\,\boldsymbol{\delta}) : \boldsymbol{S_0^S} : \boldsymbol{\delta}$$

éq 3.2.1-7

Note:

In the isotropic case the expression of the module of Biot of the solid matrix is given by:

$$\frac{1}{M_\varphi} = 3(b - \varphi)\left(\frac{1 - 2\,\nu^S}{E^S}\right)$$

- $\boldsymbol{S_0^S}$ the matrix of flexibility of the skeleton, function of the Young modulus of the solid matrix E^S and of the Poisson's ratio of the solid matrix ν^S . By supposing that microscopically the skeleton is isotropic homogeneous [12], the form of the matrix of flexibility is given by:

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 14/62
Clé : R7.01.11   Révision   :
3731397193c7

$$S_0^S = \begin{vmatrix} \dfrac{1}{E^S} & -\dfrac{\nu^S}{E^S} & -\dfrac{\nu^S}{E^S} & 0 & 0 & 0 \\[2mm] -\dfrac{\nu^S}{E^S} & \dfrac{1}{E^S} & -\dfrac{\nu^S}{E^S} & 0 & 0 & 0 \\[2mm] -\dfrac{\nu^S}{E^S} & -\dfrac{\nu^S}{E^S} & \dfrac{1}{E^S} & 0 & 0 & 0 \\[2mm] 0 & 0 & 0 & 2\dfrac{(1+\nu^S)}{E^S} & 0 & 0 \\[2mm] 0 & 0 & 0 & 0 & 2\dfrac{(1+\nu^S)}{E^S} & 0 \\[2mm] 0 & 0 & 0 & 0 & 0 & 2\dfrac{(1+\nu^S)}{E^S} \end{vmatrix} \qquad \textbf{éq 3.2.1-8}$$

In practice it is very difficult to have access to the microscopic parameters E^S and ν^S characterizing the solid matrix. We can however free us from the knowledge of these two parameters per deduction of the coefficients of compressibility of the solid matter constituents starting from the elastic parameters of the porous environment.

Taking into account what was known as previously, we chose to arbitrarily fix in the programming the value of $\nu^S = 0,3$ (cf. [12]). One adopts then the following approach in order to determine the tensor of flexibility of the solid matrix:

- it is supposed that on a microscopic scale, the solid matrix is homogeneous. Moreover it is considered that the voluminal deformation of the solid matrix between the initial moment and the final moment (after mechanical loading) is negligible. Thus the definition of the module of compressibility of the solid matter constituents is given by:

$$K_S = \frac{E^S}{3(1-2\nu^S)}$$

- expressions components of the tensor of Biot, according to the axes L and N local reference mark of orthotropism are data by [12]:

$$\begin{cases} b_L = 1 - \dfrac{M_{11} + M_{12} + M_{13}}{3\,K_S} \\[3mm] b_N = 1 - \dfrac{2M_{13} + M_{33}}{3\,K_S} \end{cases}$$

with:

$$M_{11} = \frac{E_L(E_N - E_L\nu_{LN}^2)}{(1+\nu_{LT})(E_N - E_N\nu_{LT} - 2E_L\nu_{LN}^2)}$$

$$M_{12} = \frac{E_L(E_N\nu_{LT} + E_N\nu_{LN}\nu_{LT} + E_L\nu_{LN}^2)}{(1+\nu_{LT})(E_N - E_N\nu_{LT} - 2E_L\nu_{LN}^2)}$$

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 15/62
Clé : R7.01.11   Révision   :
3731397193c7

$$M_{13} = \frac{E_L E_N \nu_{LN}}{(1+\nu_{LT})(E_N - E_N \nu_{LT} - 2 E_L \nu_{LN}^2)}$$

$$M_{33} = \frac{E_L^2(1-\nu_{LT})}{E_N - E_N \nu_{LT} - 2 E_L \nu_{LN}^2}$$

By considering one or the other of the two expressions above (taking into account the assumption of isotropy carried out on K_S), we are then able to isolate K_S.

- starting from the expression of K_S determined previously, one can have access to the Young modulus E^S solid matrix knowing that:

$$\begin{cases} \nu_S = 0,3 \\ E_S = 3(1-2\nu^S) K^S \end{cases}$$

éq 3.2.1-9

3.2.1.3 Case without mechanical coupling

For purely hydraulic or thermohydraulic modelings 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 pressure of liquid such as:

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

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

3.2.2 Evolution of the contributions of fluid mass

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

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

éq 3.2.2-1

Notice :
> *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 liquid and gas. One

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 16/62
Clé : R7.01.11   Révision   :
3731397193c7

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_{V_s} voluminal variation of the solid matter constituents.

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

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

But $\Omega(1-\varphi) = \Omega^0(1+\epsilon_V)(1-\varphi)$.
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 eulérienne definition 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 contribution in liquid:

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

One obtains:
$$\rho_s(1-\varphi)\Omega + \rho_{lq}\varphi\,\Omega = \rho_{\dot{c}s}^0(1-\varphi^0)\Omega^0 + \rho_{\dot{c}lq}^0\varphi^0\Omega^0 + m_{lq}\Omega^0$$
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 Laws of behavior of the fluids

3.2.3.1 Liquid

$$\frac{d\,\rho_w}{\rho_w} = \frac{dp_w}{K_w} - 3\,\alpha_w\,dT \qquad \textbf{éq 3.2.3.1 - 1}$$

One sees appearing the module of compressibility of water K_w and its module of dilation α_w .

3.2.3.2 Gas

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 17/62
Clé : R7.01.11   Révision :
3731397193c7

$$\frac{p_{vp}}{\rho_{vp}}=\frac{R}{M_{vp}^{ol}}T$$

éq 3.2.3.2 - 1

$$\frac{p_{as}}{\rho_{as}}=\frac{R}{M_{as}^{ol}}T$$

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 enthali

3.2.4.1   Liquid enthalpy

$$dh_w^m=C_w^p dT+\left(1-3\,\alpha_w\,T\right)\frac{dp_w}{\rho_w}$$

éq 3.2.4.1 - 1

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

By replacing in this expression the pressure of the liquid by its value according to the capillary pressure and of the pressure of gas, one a:

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

éq 3.2.4.1 - 2

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

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

éq 3.2.4.1 - 3

3.2.4.2   Enthalpy of gases

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

éq 3.2.4.2 - 1

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

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 $\delta Q^{'}$ who represents the heat received by the system except contribution enthalpic of the fluids.

$$\delta Q^{'}=\left(\boldsymbol{C_0}:\boldsymbol{\alpha_0}:\boldsymbol{d\,\varepsilon}\right)T+3\,\alpha_{lq}^m Tdp_c-\left(3\,\alpha_{gz}^m+3\,\alpha_{lq}^m\right)Tdp_{gz}+C_\varepsilon^0 dT$$

Éq 3.2.4.3 - 1

One sees appearing several dilation coefficients: $\alpha_{lq}^m,\alpha_{gz}^m$. Components of the tensor $\boldsymbol{\alpha_0}$ are data materials. In the isotropic case, the components of the tensor are equal $\left(\alpha_L=\alpha_N=\alpha_0\right)$ and correspond at the same time to the dilation coefficients of the porous environment and to those of the solid matter constituents (which are being inevitably equal in the theory that we present here).

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 18/62
Clé : R7.01.11 Révision :
3731397193c7

One also sees appearing the tensor C_0, corresponding to the matrix of Hooke of the skeleton. This tensor is function of the mechanical parameters of the porous environment $(E_L, E_N, \nu_{LT}, \nu_{LN}, G_{LN})$ in the transverse isotropic case or (E, ν) in the isotropic case.

Note:

In the isotropic case the expression of the contribution of heat except fluid is given by:

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

with K_0 the coefficient of compressibility of the porous environment, elastic function of the parameters of the porous environment (E, ν)

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

$$\alpha_{gz}^m = (1 - S_{lq}) \alpha_\varphi + \frac{\varphi (1 - S_{lq})}{3T}$$ **éq 3.2.4.3 - 2**

$$\alpha_{lq}^m = S_{lq} \alpha_\varphi + \alpha_{lq} \varphi S_{lq}$$ **éq 3.2.4.3 - 3**

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

$$C_\varepsilon^0 = C_\sigma^0 - T (C_0 : \alpha_0) : \alpha_0$$ **éq 3.2.4.3 - 4**

Note:

In the isotropic case the expression of the specific heat to constant deformation of the porous environment is given by:

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

C_σ^0 is given by a law of mixture:

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

where C_σ^s represent the specific heat to constant constraint of the constituents solid matter S and ρ_s density of the solid matter constituents. For the calculation of ρ_s, one neglects the deformation of the solid matter constituents, one thus confuses ρ_s with its initial value ρ_s^0, which is calculated in fact starting from the initial specific mass of the porous environment r_0 by the following formula of the mixtures:

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

3.2.5 Laws of diffusion (complementary laws)

3.2.5.1 Diffusion of heat

One takes the classical law of Furrier:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 19/62
Clé : R7.01.11   Révision   :
3731397193c7

$$\mathbf{q} = -\boldsymbol{\lambda}^T . \nabla T$$

éq 3.2.5.1 - 1

where one sees appearing the thermal tensor of conductivity $\boldsymbol{\lambda}^T$.

The tensor of conductivity is function of porosity, saturation and the temperature and is given in the shape of the product of three functions plus a constant:

$$\boldsymbol{\lambda}^T = \lambda_\varphi^T(\phi) . \lambda_S^T(S_{lq}) . \boldsymbol{\lambda}_T^T(T) + \boldsymbol{\lambda}_{cte}^T$$

éq 3.2.5.1 - 2

In the isotropic case, one has $\boldsymbol{\lambda}^T = \lambda^T . \mathbf{1}$, $\boldsymbol{\lambda}_T^T(T) = \lambda_T^T(T) . \mathbf{1}$ and $\boldsymbol{\lambda}_{cte}^T = \lambda_{cte}^T . \mathbf{1}$.

3.2.5.2 Diffusion of the fluids

They are the laws of Darcy, to which one adds the law of Fick in the presence of vapor.
The laws of Darcy are written for gas and the liquid:

$$\frac{\mathbf{M}_{lq}}{\rho_{lq}} = \boldsymbol{\lambda}_{lq}^H \left(-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m \right)$$

éq 3.2.5.2 - 1

$$\frac{\mathbf{M}_{gz}}{\rho_{gz}} = \boldsymbol{\lambda}_{gz}^H \left(-\nabla p_{gz} + \rho_{gz} \mathbf{F}^m \right)$$

éq 3.2.5.2 - 2

where we see appearing the tensors of hydraulic conductivity $\boldsymbol{\lambda}_{lq}^H$ and $\boldsymbol{\lambda}_{gz}^H$ for the liquid and gas respectively. In the isotropic cases, $\boldsymbol{\lambda}_{lq}^H = \lambda_{lq}^H . \mathbf{1}$ and $\boldsymbol{\lambda}_{gz}^H = \lambda_{gz}^H . \mathbf{1}$.

One makes the approximation that $\dfrac{\mathbf{M}_w}{\rho_w} = \boldsymbol{\lambda}_w^H \left(-\nabla p_{lq} + \rho_{lq} \mathbf{F}^m \right)$.

Note:

In this expression of the law of Darcy, one neglects the differential acceleration of water. In the case of very permeable and very porous mediums subjected to a seismic loading, that can constitute a limit.

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

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

éq 3.2.5.2 - 3

where D_{vp} is the coefficient of diffusion of Fick of the gas mixture (L^2. T^{-1}), one notes thereafter F_{vp} such as:

$$F_{vp} = \frac{D_{vp}}{C_{vp}(1 - C_{vp})}$$

éq 3.2.5.2 - 4

and with

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 *Page : 20/62*
Clé : R7.01.11   *Révision   :*
3731397193c7

$$C_{vp} = \frac{p_{vp}}{p_{gz}}$$

éq 3.2.5.2 - 5

One thus has:

$$\frac{\mathbf{M}_{vp}}{\rho_{vp}} - \frac{\mathbf{M}_{as}}{\rho_{as}} = -F_{vp}\nabla C_{vp}$$

éq 3.2.5.2 - 6

Moreover, one a:

$$\frac{\mathbf{M}_{gz}}{\rho_{gz}} = \left(1 - C_{vp}\right)\frac{\mathbf{M}_{as}}{\rho_{as}} + C_{vp}\frac{\mathbf{M}_{vp}}{\rho_{vp}}$$

éq 3.2.5.2 - 7

and:

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

éq 3.2.5.2 - 8

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

$$\mathbf{M}_{ad} - \mathbf{M}_w = -D_{ad}\nabla\rho_{ad}$$

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 thereafter F_{ad} such as:

$$F_{ad} = D_{ad}$$

éq 3.2.5.2 - 10

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

$$C_{ad} = \rho_{ad}$$

éq 3.2.5.2 - 11

$$\mathbf{M}_{ad} - \mathbf{M}_w = -F_{ad}\nabla C_{ad}$$

éq 3.2.5.2 - 12

Concerning the liquid, it was admitted that the liquid law of Darcy applies at the speed of liquid water. There is not thus to define mean velocity of the liquid.

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

éq 3.2.5.2 - 13

and:

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

éq 3.2.5.2 - 14

By combining these relations, one finds then:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 21/62
Clé : R7.01.11   Révision :
3731397193c7

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

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

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

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

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

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

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

K^{int} is the tensor of intrinsic permeability, characteristic of the porous environment and user datum, unspecified function of porosity. In the isotropic case, $K^{int} = K^{int} \cdot \mathbf{1}$;

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 relative permeability with the liquid, characteristic of the porous environment and user datum, unspecified function of saturation in liquid;

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

Note:

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

The relation between the tensors 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 the derivative compared to steam pressure and saturation. Same manner 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 the derivative according to the temperature.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 22/62
Clé : R7.01.11   Révision   :
3731397193c7

3.2.6   Water-steam balance

This relation is essential and it results in to reduce it many unknown factors of pressure.
One notes h_w^m mass enthalpy of water, s_w^m its entropy and $g_w^m = h_w^m - Ts_w^m$ its free enthalpy.
One notes h_{vp}^m mass enthalpy of the vapor, s_{vp}^m its entropy and $g_{vp}^m = h_{vp}^m - Ts_{vp}^m$ its free enthalpy.
Balance water vapor is written:

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

Who gives:

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

In addition, the definition of the free enthalpy teaches us that: $dg = \dfrac{dp}{\rho} - sdT$, which, applied to the

vapor and water, compound with the relation $dg_{vp}^m = dg_w^m$ and while using [éq 3.2.6-2] gives:

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

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

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

3.2.7   Balance air dissolved dryness-air

The dissolved air is defined via the constant of Henry K_H, which connects the molar concentration
of dissolved air C_{ad}^{ol} ($moles/m^3$) with the air pressure dryness:

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

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

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 law of perfect gas:

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

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

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

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 23/62
Clé : R7.01.11 Révision :
3731397193c7

3.2.8 The mechanical behavior

One will write it in differential form:

$$d\,\sigma = d\,\sigma' + d\,\sigma_p \qquad \text{éq 3.2.8-1}$$

In the case general (except law 'HYDR_TABBAL'), EN using a formulation of Bishop [10] extended to the unsaturated mediums one writes:

$$d\,\sigma_p = -\boldsymbol{B}(dp_{gz} - S_{lq}\,dp_c) \qquad \text{éq 3.2.8-2}$$

(which corresponds well in the case saturated to the classical formulation with Biot $d\,\sigma_p = -\boldsymbol{B}\,dp_{lq}$).

One thus sees appearing in the formula [éq 3.2.8-2], the tensor of Biot. In the isotropic case $\boldsymbol{B} = b\,.\,\boldsymbol{1}$ and $\boldsymbol{\sigma}_p = \sigma_p\,.\,\boldsymbol{1}$.

This formulation is valid for "reasonable" ranges of drying, namely of the relative humidities (or degree of hygroscopy) HR understood between 50 % and 100 %. It is pointed out that the relative humidity HR and the capillary pressure are connected by the law of Kelvin (cf section 3.3).

For ranges of humidities relative going down to the lower part from 50 %, the model resulting from the thesis of Ginger El Tabbal [14] is recommended. This model is called by keyword HYDR_TABBAL under RELATION_KIT. Besides the capillary action used in the formulation above, the effect of adsorption is taken here into account. In this case, the hydraulic constraint is written in the form $d\,\sigma_p = -\boldsymbol{B}\,d\,\pi$ hasvec:

$$d\,\pi = dp_{gz} - S_{BJH}\,dp_c - \frac{1}{3}\,p_c(S_{BJH})dS_{BJH}$$

$$+ \frac{2}{3}(A_0/\phi^0)(-(\omega_{BJH}(S_{BJH})dt(HR) + t(HR)d\,\omega_{BJH}(S_{BJH}))\,.\,dp_c - \left(\frac{\partial\gamma}{\partial\varepsilon_s}\right)\Bigg|_\mu d\,\omega_{BJH}(S_{BJH}))$$

$$\text{éq 3.2.8-3}$$

With S_{BJH} , A_0 , ω_{BJH} , $t(HR)$ and $\left(\dfrac{\partial\gamma}{\partial\varepsilon_s}\right)\Bigg|_\mu$ data input of the model calculated as a preliminary.

One gives the definition here of it:

S_{BJH} Voluminal fraction of liquid water function of HR (not adsorbed water). This function is calculated by method BJH [16].

A_0 Entire surface of the pores (or surfaces specific materials) by unit of volume m ^{2} /m^3. It is the product of the density dries (g/m^3) material by the specific surface (m ^{2} /g) determined by method Study Bureau [17] or BJH [16].

ω_{BJH} Surface fraction of the unsaturated pores Foiling of relative humidity HR. It is the relationship between the surface of the unsaturated pores (by unit of volume) determined by the method BJH (with a given relative moisture) and the entire surface of the pores A_0 .

$t(HR)$ Thickness of the layer of adsorbed water. This thickness is evaluated by an empirical relation known as of Badmann [15] .

$\left(\dfrac{\partial\gamma}{\partial\varepsilon_s}\right)\Bigg|_\mu$ Term of Shuttleworth, strongly depend on directedTion and of the morphology of solid

surface. This term is readjusted with to start from experiment of withdrawal of drying.

S_{BJH} , A_0 , ω_{BJH} , are thus calculated starting from experimental data by said digital methods Study Bureau or BJH. Methodology to obtain these parameters as well as the thickness of the adsorbed layer and the parameter of Shuttleworth is described in detail in Doc. U2.04.05.

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 24/62
Clé : R7.01.11   Révision   :
3731397193c7

In the relation [éq 3.2.8-1] evolution of the tensor of effective constraint σ' is supposed to depend only on the displacement of the skeleton and internal variables α. The usual terms related to the thermal deformation are integrated into the calculation of the effective constraint:

$$d\,\sigma\,'=f\big(d\,\varepsilon-\alpha_0\,dT\,\mathbf{I}\,,d\,\alpha\big)$$

éq 3.2.8-4

The reason of this choice is to be able to use any law of classical thermomechanics for the calculation of the effective constraints, laws which, in more the share of the writings are in conformity with [éq 3.2.8-3].

In practice, Lhas thermal deformation is evaluated by the following formula:

$$\varepsilon^{th}\big(T\big)=\alpha_0\big(T-T_{ini}\big)$$

(1)

The temperature of reference is given by `THM_INIT/TEMP` in `DEFI_MATERIAU`.

3.2.9 Precise details on the diphasic terms of transfers

3.2.9.1 The isotherm of sorption

To close the system, there remains still a relation to be written, connecting saturation and the pressures. We chose to consider that saturation in liquid 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 very well $S_{lq}\big(p_c\big)$ refine per pieces, and since the derivative of this function, $\dfrac{\partial S_{lq}}{\partial p_c}$, 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 hard" 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 ways of drying and the ways 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 tabulée form, relative permeabilities, laws of saturation and their derivative while making sure of their coherence (keyword `HYDR_UTIL` or `HYDR_TABBAL` under `RELATION_KIT`), that is to say to make call to a model known and programmed in analytical form: the model Mualem – Van Genuchten (keyword `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 is currently not available in Aster. It is then to the user to return them in form tabulée in the command file. The model Mualem- Van Genuchten is a classical model for the description of 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 law capillary saturation/pressure (Van Genuchten to which one adds a pressure of entry) such as:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 25/62
Clé : R7.01.11   Révision :
3731397193c7

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

with $\quad S_{we} = \cfrac{S - S_{wr}}{1 - S_{wr}} \quad$ and $\quad m = 1 - \cfrac{1}{n}$

n, S_{wr} (residual water saturation) and P_r are parameters of the models indicated by the user in his command file. P_e is also a parameter (by default taken equal to 0) correspondent with a pressure of entry (the medium désature only if the capillary pressure is higher than this pressure.

The permeability relating to water is expressed then by integrating the model of 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 to 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 law in the case of it `HYDR_VGC` :

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

In *Code_hasster*, 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 treatment which one carries out on these curves, $Smax$ and $CSAT$:

For $S > Smax$, these curves are interpolated by a polynomial of degree 2 $C1$ in $Smax$, so as to avoid having to treat derivative of infinite values. Indeed, for $S=1$:

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

and for the case `HYDR_VGM` $\quad \dfrac{\partial k_r^{gz}(S)}{\partial S} = \infty$

To avoid having then to deal with this problem (which does not have a priori physical meaning) one replaces these functions starting from a saturation $Smax$ by a polynomial of the second order C^1 in this point.

What gives for the function $k_r^w(S)$:
For $S = Smax$, the polynomial is determined $PL(S)$ such as:

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

For $S > Smax$, $k_r^w(S)$ is replaced by $PL(S)$.
And for $k_r^{gz}(S)$ in the case `HYDR_VGM` :
For $S = Smax$, the polynomial is determined $PG(S)$ such as:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 26/62
Clé : R7.01.11 Révision : 3731397193c7

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

For $S>Smax$, $k_r^{gz}(S)$ is replaced by $PG(S)$.

For suction $S(Pc)$ and for $Pc<Pcmin$ (with $S(Pcmin)=Smax$) the curve is prolonged $S(Pc)$ by a hyperbole such as the curve is C^1 in this point:
For $S>Smax$:

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

with A and B such that the curve is $C1$ in $Smax$.

There is thus well a decreasing curve which tends towards 1 when Pc tends towards $-\infty$. This treatment 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).

$S(Pc)$ 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 material and the user data

- drained Young moduli E_L and E_N as well as the drained Poisson's ratios ν_{LT} and ν_{LN} who allow the calculation of the matrix of flexibility of the porous environment. (transverse isotropic case),
- the drained Young modulus E, and the drained Poisson's ratio ν who allow the calculation of the matrix of flexibility of the porous environment. (isotropic case),
- average coefficients of Biot b_L and b_N who allow the calculation of the module of Biot of the solid matrix $\dfrac{1}{M_\varphi}$ (transverse isotropic case),
- the coefficient of Biot $b=1-\dfrac{K_0}{K_S}$ allows to calculate the module of compressibility of the solid matter constituents K_S, useful in the calculation of porosity for the isotropic case,
- the module of compressibility of water K_w,
- the dilation coefficient of water α_w,
- the constant of perfect gases R,
- molar mass of the vapor M_{vp}^{ol},
- molar mass of the dry air M_{as}^{ol}, (= M_{ad}^{ol})
- specific heat with constant pressure of water C_w^p,
- specific heat with constant pressure of the dissolved air C_{ad}^p
- specific heat with constant pressure of the dry air C_{as}^p,
- specific heat with constant pressure of the vapor C_{vp}^p,
- average dilation coefficients of the porous environment α_L and α_N, which is also those of the solid matter constituents. They allow the calculation of α_φ (transverse isotropic case),
- the dilation coefficient of the porous environment α_0, which is also that of the solid matter constituents. It allows the calculation of $\alpha_\varphi=(b-\varphi)\alpha_0$ (isotropic case),

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 27/62
Clé : R7.01.11 Révision : 3731397193c7

- specific heat with constant constraint of the solid matter constituents C_σ^s ,
- the thermal tensor of conductivity of the solid matter constituents only, λ_s^T , unspecified function of the temperature,
- the thermal tensor of conductivity of the liquid, λ_{lq}^T , unspecified function of the temperature,
- the thermal tensor of 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 temperature and the pressure of liquid, the pressure of the dissolved air and saturation.
- The constant of Henry K_H unspecified function of the temperature,
- the intrinsic tensor of permeability, $\boldsymbol{K}^{\mathbf{int}}$, 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 liquid, k_{lq}^{rel} , unspecified function of saturation in liquid,
- the permeability relating to gas, k_{gz}^{rel} , fonunspecified ction of saturation in liquid and the gas pressure,
- the relation capillary saturation/pressure, $S_{lq}(p_c)$, unspecified function of the capillary pressure,
- in a general way the initial state is characterized by:
  - the initial temperature,
  - initial pressures from where initial saturation is deduced $S_{lq}^0\left(p_c^0\right)$,
  - 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 the dry air ρ_{as}^0 .
  - homogenized initial density porous environment r_0 ,

  - initial enthali of water, the dissolved air, the vapor and the 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 enthali.
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 enthali are worthless,
- 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 enthali of water and vapor one will have to take:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 28/62
Clé : R7.01.11   Révision   :
3731397193c7

$$^{init}h_w^m = \frac{p_w^{init} - p_l^{ref}}{\rho_w} = \frac{p_w^{init} - p_{atm}}{\rho_w}$$

$$^{init}h_{vp}^m = L(T^{init}) = \text{chaleur latente de vaporisation}$$

$$^{init}h_{as}^m = 0$$

$$^{init}h_{ad}^m = 0$$

Note:

The initial vapor pressure must be taken in coherence with 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 at the temperature considered. One then uses the law of Kelvin which gives the pressure of the liquid according to the steam pressure, of the temperature and the saturating steam

pressure: $\dfrac{p_w - p_w^{ref}}{\rho_w} = \dfrac{R}{M_{vp}^{ol}} T \ln\left(\dfrac{p_{vp}}{p_{vp}^{sat}(T)}\right)$. *This relation is valid only for isothermal*

evolutions. It is stressed that p_w^{ref} *corresponds in a state of 'balance to which*

corresponds p_{vp}^{sat} *, this state of balance corresponds in fact to* $p_w^0 = p_{gz}^0 = 1$ *atm. For*

evolutions with temperature variation, knowing a law giving the steam pressure

saturating *to* *the* *temperature* T_0 *,* *for* *example:*

$p_{vp}^{sat}(T_0) = 10^{\left(2.7858 + \frac{T_0 - 273.5}{31.559 + .1354(T_0 - 273.5)}\right)}$ *, 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 unknown factors, 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 unknown factors which are also the values of the degrees of freedom, are noted:

$$[u]^{ddl} = \begin{Bmatrix} u_x \\ u_y \\ u_z \\ PRE1^{ddl} \\ PRE2^{ddl} \\ T^{ddl} \end{Bmatrix}$$

According to modeling, they can have different meanings:

	LIQU_SATU	LIQU_VAPE	LIQU_GAZ_ATM	GAS	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:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 29/62
Clé : R7.01.11   Révision   :
3731397193c7

$p = p^{ddl} + p^{init}$ for the pressures PRE1 and PRE2 and $T = T^{ddl} + T^{init}$ for the temperatures, where p^{init} and T^{init} are defined under the keyword THM_INIT order DEFI_MATERIAU. Values written by IMPR_RESU are the values of $\lfloor u \rfloor^{ddl}$. The boundary conditions are defined for $\lfloor u \rfloor^{ddl}$. The keyword DEPL keyword factor ETAT_INIT order STAT_NON_LINE defines the initial values of $\lfloor u \rfloor^{ddl}$. Initial values of the enthali, which belong to the generalized constraints are defined starting from the keyword SIGM keyword factor ETAT_INIT order STAT_NON_LINE. The real pressures and the real temperature are used in the laws of behavior, in particular the laws of the type $S_{lq} = f(p_c)$ or $\dfrac{dp}{p} = \dfrac{d\rho}{\rho} + \dfrac{dT}{T}$. 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 the keyword THM_INIT order DEFI_MATERIAU). It is noticed that, for displacements, the decomposition $u = u^{ddl} + u^{init}$ is not made: the keyword THM_INIT order DEFI_MATERIAU thus does not allow to define initial displacements. The only way of initializing displacements is thus to give them an initial value by the keyword factor ETAT_INIT order STAT_NON_LINE.

3.5 Effective constraints and total constraints. Boundary conditions of contrainteLa partition of the constraints in constraints total and effective is written:

$$\sigma = \sigma' + \sigma_p$$

σ is the total constraint, c.a.d that which checks: $\mathbf{Div}(\sigma) + r\,\mathbf{F}^m = 0$

σ' is the effective constraint. For the laws of effective constraints, it checks: $d\,\sigma' = f(d\,\varepsilon - \alpha_0\,dT, \alpha)$, where $\varepsilon = 1/2(\nabla\mathbf{u} + {}^T\nabla\mathbf{u})$ and α represent the internal variables. The tensor σ_p is calculated according to the water pressures. The adopted writing is incremental and, if it is wanted that the value of σ_p that is to say coherent with the value p^{init} defined under the keyword THM_INIT, it is necessary to initialize the components of σ_p by the keyword SIGM keyword factor ETAT_INIT order STAT_NON_LINE.

In the files results, one finds the constraints effective σ' under the names of components SIXX … and σ_p under the name SIPXX … . The boundary conditions in constraints are written in total constraints.

3.6 Some digital 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:

$$R = 8.3144 \; J.K^{-1}$$
$$M_{vp}^{ol} = 18.\ 10^{-3}\, kg.mole^{-1}$$
$$M_{as}^{ol} = 28.96\,10^{-3}\, kg.mole^{-1}$$

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

$$K_H = 3162\, Pa.m^3 mole^{-1}$$

For liquid water, one a:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 30/62
Clé : R7.01.11   Révision   :
3731397193c7

$$\rho_w = 1000 \ kg/m^3$$
$$K_w = 2000 \ MPa$$

The thermal dilation coefficient of water is correctly approached by the formula:

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

The heat-storage capacities have as values:

$$C_\sigma^s = 800 \ J.kg^{-1} K^{-1}$$
$$C_{lq}^p = 4180 \ J.kg^{-1} K^{-1}$$
$$C_{vp}^p = 1870 \ J.kg^{-1} K^{-1}$$
$$C_{as}^p = 1000 \ J.kg^{-1} K^{-1}$$

To a law of evolution of the latent heat of liquid phase shift vapor is also given:
$$L(T) = 2500800 - 2443(T - 273.15) \ J/kg$$

4 Calculation of the generalized constraints

In this chapter, we specify how are integrated the relations described into chapter 3. More precisely still, we give the expressions of the constraints generalized within the meaning of the document [R7.01.10] [4] when laws of behaviors THM are called for the option RAPH_MECA within the meaning of the document [R5.03.01] [3]. So that this document follows of readier the order of programming, we will consider two cases: the case without dissolved air and that with.

The generalized constraints are:

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

The generalized deformations, from which the generalized constraints are calculated are:

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

The internal variables that 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 the step of time and the indices - for the quantities at the beginning of the step of time.

Thus, the known quantities are:

• generalized constraints, deformations and internal variables at the beginning of the step of time:
  • $\sigma'^-, \sigma_p^- ; m_w^-, \mathbf{M}_w^-, h_w^{m-} ; m_{vp}^-, \mathbf{M}_{vp}^-, h_{vp}^{m-} ; m_{as}^-, \mathbf{M}_{as}^-, h_{as}^{m-} ; m_{ad}^-, \mathbf{M}_{ad}^-, h_{ad}^{m-} ; Q^{r-}, \mathbf{q}^-$
  • $\mathbf{u}^-, \varepsilon(\mathbf{u}^-) ; p_c^-, \nabla p_c^- ; p_{gz}^-, \nabla p_{gz}^- ; T^-, \nabla T^-$
  • $\varphi^-, \rho_w^-, p_{vp}^-, p_{ad}^-$

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 31/62
Clé : R7.01.11 Révision :
3731397193c7

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

4.1 Case without dissolved air

4.1.1 Calculation of porosity and it density of the fluid

4.1.1.1 Calculation of porosity: isotropic case

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

One obtains then:

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

4.1.1.2 Calculation of porosity: transverse isotropic case

The first thing to be made is of course to calculate saturation at the end of the step of time $S_{lq}^+ = S_{lq}(p_c^+)$. Porosity is by integrating on the step of time the equation [éq 3.2.1-3]. Integration is thus here explicit contrary to the isotropic case.
One obtains then:

$$(\varphi^+ - \varphi^-) = \boldsymbol{B}:(\varepsilon^+ - \varepsilon^-) - \varphi^-(\varepsilon_v^+ - \varepsilon_v^-) - 3\alpha_\varphi(T^+ - T^-) + \frac{(p_{gz}^+ - p_{gz}^-) - S_{lq}^+(p_c^+ - p_c^-)}{M_\varphi} \qquad \textbf{éq 4.1.1-2}$$

4.1.1.3 Calculation of the density of the fluid

The density of the liquid is by integrating on the step of time the equation [éq 3.2.3.1 - 1].

What gives:

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

4.1.2 Calculation of the dilation coefficients

It is important to notice that the thermal dilation coefficient differential is recomputed starting from the porosity evaluated at the end of the step of time. Taking into account that one poses:

$$\alpha_\varphi^+ = \frac{(\boldsymbol{B} - \varphi^+\boldsymbol{\delta}):\alpha_0}{3} \qquad \textbf{éq 4.1.2-1}$$

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 32/62
Clé : R7.01.11   Révision   :
*   3731397193c7*

Note:

In the isotropic case [éq 4.1.2-1] becomes:

$$\alpha_{\varphi}^{+} = (b - \varphi^{+}) \alpha_0$$

It is then about 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 the step of time:

$$\alpha_{vp}^{m^{+}} = \alpha_{as}^{m^{+}} = \alpha_{gz}^{m^{+}} = (1 - S_{lq}^{+}) \alpha_{\varphi}^{+} + \frac{\varphi^{+}(1 - S_{lq}^{+})}{3 T^{+}} \qquad \text{éq 4.1.2-2}$$

$$\alpha_{w}^{m^{+}} = S_{lq}^{+} \alpha_{\varphi}^{+} + \alpha_{lq} \varphi^{+} S_{lq}^{+} \qquad \text{éq 4.1.2-3}$$

4.1.3 Calculation of the fluid enthali

The fluid enthali 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].

$$h_{w}^{m^{+}} = h_{w}^{m^{-}} + C_{w}^{p}(T^{+} - T^{-}) + \frac{(1 - 3 \alpha_{w} T^{+})}{\rho_{w}^{+}} (p_{gz}^{+} - p_{gz}^{-} - p_{c}^{+} + p_{c}^{-}) \qquad \text{éq 4.1.3-1}$$

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

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

4.1.4 Air and steam pressures

On the basis of the relation [éq 3.2.6-4] in which one carries the law of reaction of perfect gases [éq 3.2.3.2 - 1], one finds $\dfrac{dp_{vp}}{p_{vp}} = \dfrac{M_{vp}^{ol}}{RT}\left(\dfrac{1}{\rho_w} dp_{gz} - \dfrac{1}{\rho_w} dp_c + (h_{vp}^m - h_w^m)\dfrac{dT}{T}\right)$ that one integrates by a

way initially into constant temperature (one then considers the density of constant water), then of T^{-} with T^{+} with constant pressures.

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

The first term corresponds to the way at constant temperature, the second with the way with constant pressures. By using the definitions [éq 3.2.4.1 - 1] and [éq 3.2.4.2 - 1] of the enthali, one sees 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 way:

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 33/62
Clé : R7.01.11 Révision :
3731397193c7

That is to say finally:

$$\ln\left(\frac{p_{vp}^+}{p_{vp}^-}\right)=\frac{M_{vp}^{ol}}{RT^+}\frac{1}{\rho_w^+}\left[\left(p_{gz^+}-p_{gz}^-\right)-\left(p_{c^+}-p_c^-\right)\right]+$$

$$\frac{M_{vp}^{ol}}{R}\left(h_{vp}^{m^-}-h_w^{m^-}\right)\left(\frac{1}{T^-}-\frac{1}{T^+}\right)+\frac{M_{vp}^{ol}}{R}\left(C_{vp}^p-C_w^p\right)\left(\ln\left(\frac{T^+}{T^-}\right)+\frac{T^-}{T^+}-1\right)$$

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]:

$$\rho_{vp}^+=\frac{M_{vp}^{ol}}{R}\frac{p_{vp}^+}{T^+}$$

éq 4.1.4-2

$$\rho_{as}^+=\frac{M_{as}^{ol}}{R}\frac{\left(p_{gz}^+-p_{vp}^+\right)}{T^+}$$

éq 4.1.4-3

4.1.5 Calculation of the mass contributions

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

$$m_w^+=m_w^-+\rho_w^+\left(1+\varepsilon_V^+\right)\varphi^+S_{lq}^+-\rho_w^-\left(1+\varepsilon_V^-\right)\varphi^-S_{lq}^-$$
$$m_{as}^+=m_{as}^-+\rho_{as}^+\left(1+\varepsilon_V^+\right)\varphi^+(1-S_{lq}^+)-\rho_{as}^-\left(1+\varepsilon_V^-\right)\varphi^-(1-S_{lq}^-)$$
$$m_{vp}^+=m_{vp}^-+\rho_{vp}^+\left(1+\varepsilon_V^+\right)\varphi^+(1-S_{lq}^+)-\rho_{vp}^-\left(1+\varepsilon_V^-\right)\varphi^-(1-S_{lq}^-)$$

éq 4.1.5-1

4.1.6 Calculation of the heat-storage capacity and Q' heat

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

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

éq 4.1.6-1

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

$$C_\varepsilon^{0^+}=C_\sigma^{0^+}-T^+(\boldsymbol{C_0}:\boldsymbol{\alpha_0}):\boldsymbol{\alpha_0}$$

éq 4.1.6-2

Note:

In the isotropic case [éq 4.1.6-2] becomes:

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

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021   Page : 34/62
Clé : R7.01.11   Révision   :
3731397193c7

$$Q'^{+}=Q'^{-}+(C_0:\alpha_0):\left(\varepsilon^{+}-\varepsilon^{-}\right)T^{1/2}+3\alpha_{lq}^{m^+}T^{1/2}\left(p_c^{+}-p_c^{-}\right)-\left(3\alpha_{gz}^{m^+}+3\alpha_{lq}^{m^+}\right)T^{1/2}\left(p_{gz}^{+}-p_{gz}^{-}\right)+C_{\varepsilon}^{0^+}\left(T^{+}-T^{-}\right)$$

éq 4.1.6-3

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

Note:

In the isotropic case [éq 4.1.6-3] becomes:

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

4.1.7 Calculation of the mechanical constraints

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

$$\sigma_p^{+}=\sigma_p^{-}-B\left(p_{gz}^{+}-p_{gz}^{-}\right)+B\,S_{lq}^{+}\left(p_c^{+}-p_c^{-}\right)$$

éq 4.1.7-1

In the isotropic case one has $B=b.1$, $\sigma_p^{+}=\sigma_p^{+}.1$ and $\sigma_p^{-}=\sigma_p^{-}.1$

4.1.8 Calculation of hydrous and thermal flows

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

The coefficient of Fick $F^{+}=F\left(T^{+},p_c^{+},p_{gz}^{+}\right)$

The thermal tensor of diffusivity $\lambda^{T+}=\lambda_{\phi}^{T}\left(\varphi^{+}\right).\lambda_S^{T}\left(S_{lq}^{+}\right).\lambda_T^{T}\left(T^{+}\right)+\lambda_{cte}^{T}$

Tensors of permeability and hydraulic conductivity:

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

In the isotropic case, $K^{int}=K^{int}.1$, $\lambda^{T}=\lambda^{T}.1$, $\lambda_T^{T}(T)=\lambda_T^{T}(T).1$ and $\lambda_{cte}^{T}=\lambda_{cte}^{T}.1$

Vapor concentrations: $C_{vp}^{+}=\dfrac{p_{vp}^{+}}{p_{vp}^{+}}$

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:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 35/62
Clé : R7.01.11 Révision :
3731397193c7

$$\mathbf{q}^{+} = -\lambda^{T^{+}} \nabla T^{+}$$

éq 4.1.8-1

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

éq 4.1.8-2

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

éq 4.1.8-3

$$\frac{\mathbf{M}_{w}^{+}}{\rho_{w}^{+}} = \lambda_{lq}^{H^{+}} \left[-\nabla p_{lq}^{+} + \rho_{w}^{+} F^{m} \right]$$

éq 4.1.8-4

In the isotropic cases, $\lambda_{lq}^{H} = \lambda_{lq}^{H} . \mathbf{1}$ and $\lambda_{gz}^{H} = \lambda_{gz}^{H} . \mathbf{1}$.

4.2 Case with dissolved air

4.2.1 Calculation of porosity

4.2.1.1 Calculation of porosity: isotropic case

Same manner, the first thing to be made is to calculate saturation at the end of the step of time $S_{lq}^{+} = S_{lq}\left(p_{c}^{+} \right)$. Porosity is by integrating on the step of time the equation [éq 3.2.1-1]. It is thus pointed out that:

$$\ln \left\{ \frac{b - \varphi^{+}}{b - \varphi^{-}} \right\} = \left\{ -\left(\varepsilon_{v}^{+} - \varepsilon_{v}^{-} \right) + 3 \alpha_{0} \left(T^{+} - T^{-} \right) - \frac{\left(p_{gz}^{+} - p_{gz}^{-} \right) - S_{lq}^{+} \left(p_{c}^{+} - p_{c}^{-} \right)}{K_{S}} \right\}$$

4.2.1.2 Calculation of porosity: transverse isotropic case

Same manner, the first thing to be made is to calculate saturation at the end of the step of time $S_{lq}^{+} = S_{lq}\left(p_{c}^{+} \right)$. Porosity is by integrating on the step of time the equation [éq 3.2.1-1]. It is thus pointed out that:

$$\left(\varphi^{+} - \varphi^{-} \right) = \boldsymbol{B} : \left(\boldsymbol{\varepsilon}^{+} - \boldsymbol{\varepsilon}^{-} \right) - \varphi^{-} \left(\varepsilon_{v}^{+} - \varepsilon_{v}^{-} \right) - 3 \alpha_{\varphi} \left(T^{+} - T^{-} \right) + \frac{\left(p_{gz}^{+} - p_{gz}^{-} \right) - S_{lq}^{+} \left(p_{c}^{+} - p_{c}^{-} \right)}{M_{\varphi}}$$

4.2.2 Calculation of the dilation coefficients

Same manner, the thermal dilation coefficient differential is recomputed starting from the porosity evaluated at the end of the step of time. Taking into account that one poses:

$$\alpha_{\varphi}^{+} = \frac{\left(\boldsymbol{B} - \varphi^{+} \boldsymbol{\delta} \right) : \alpha_{0}}{3}$$

éq 4.2.2-1

Note:

In the isotropic case [éq 4.2.2-1] becomes:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 36/62
Clé : R7.01.11 Révision :
3731397193c7

$$\alpha_\varphi^+ = (b - \varphi^+)\alpha_0$$

It is then about 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 the step of time:

$$\alpha_{vp}^{m^+} = a_{as}^{m+} = a_{gz}^{m+} = \left(1 - S_{lq}^+\right)\alpha_\varphi^+ + \frac{\varphi^+\left(1 - S_{lq}^+\right)}{3T^+} \qquad \text{éq 4.2.2-2}$$

$$\alpha_w^{m^+} = S_{lq}^+ \alpha_\varphi^+ + \alpha_{lq}\,\varphi^+\,S_{lq}^+ \qquad \text{éq 4.2.2-3}$$

$$\alpha_{ad}^{m^+} = S_{lq}^+ \alpha_\varphi^+ + \frac{\varphi^+\,S_{lq}^+}{3T^+} \qquad \text{éq 4.2.2-4}$$

4.2.3 Calculation 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 law of reaction of perfect gases [éq 3.2.3.2 - 1], one finds:

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

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

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

thus:

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

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

$$\ln\left(\frac{p_{vp}^+}{p_{vp}^-}\right) = \frac{M_{vp}^{ol}}{\rho_w^-}(\frac{1}{RT^+} - \frac{1}{K_H})\left(p_{gz^+} - p_{gz}^-\right) + \frac{M_{vp}^{ol}}{\rho_w^- K_H}\left(p_{vp^+} - p_{vp}^-\right) - \frac{M_{vp}^{ol}}{\rho_w^- RT^+}\left(p_{c^+} - p_c^-\right) +$$

$$\frac{M_{vp}^{ol} R}{\rho_w^- K_H}\left(p_{vp^+} - p_{gz}^+\right)\ln\left(\frac{T^+}{T^-}\right) + \frac{M_{vp}^{ol}}{R}\int_{T^-}^{T^+}\left(h_{vp}^m - h_w^m\right)\frac{dT}{T^2} \qquad \text{éq 4.2.3-3}$$

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 *Page : 37/62*
Clé : R7.01.11 *Révision :*
3731397193c7

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

éq 4.2.3-4

and thus

$$\tilde{p}_{vp} = p_{vp}^-.\exp\left(\frac{M_{vp}^{ol}}{\rho_w^-}\left(\frac{1}{RT^+} - \frac{1}{K_H}\right)\left(p_{gz^+} - p_{gz}^-\right) - \frac{M_{vp}^{ol}}{\rho_w^- RT^+}\left(p_{c^+} - p_c^-\right) + \int_{T^-}^{T^+}\left(h_{vp}^m - h_w^m\right)\frac{dT}{T^2}\right)$$ **éq 4.2.3-5**

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

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

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 $\ln\left(\frac{p_{vp}^+}{\tilde{p}_{vp}}\right) = \ln\left(1 + \frac{p_{vp}^+ - \tilde{p}_{vp}}{\tilde{p}_{vp}}\right) \approx \frac{p_{vp}^+}{\tilde{p}_{vp}} - 1$,

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

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

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 are 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]:

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 38/62
Clé : R7.01.11   Révision :
3731397193c7

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

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

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

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

What gives:

$$\ln\left(\frac{\rho_{w}^{+}}{\rho_{w}^{-}} \right) = \frac{p_{gz}^{+} - p_{gz}^{-} - p_{c}^{+} + p_{c}^{-} - p_{ad}^{+} + p_{ad}^{-}}{K_{w}} - 3\,\alpha_{w}\left(T^{+} - T^{-} \right) \qquad \text{éq 4.2.3-11}$$

4.2.4 Calculation of the fluid enthali

The fluid enthali 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].

$$h_{w}^{m^{+}} = h_{w}^{m^{-}} + C_{w}^{p}\left(T^{+} - T^{-} \right) + \frac{\left(1 - 3\,\alpha_{w} T^{+} \right)}{\rho_{w}^{+}} \left(p_{gz}^{+} - p_{gz}^{-} - p_{c}^{+} + p_{c}^{-} - p_{ad}^{+} + p_{ad}^{-} \right) \qquad \text{éq 4.2.4-1}$$

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

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

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

4.2.5 Calculation of the mass contributions

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

$$
\begin{aligned}
m_{w}^{+} &= m_{w}^{-} + \rho_{w}^{+}\left(1 + \varepsilon_{V}^{+} \right)\varphi^{+} S_{lq}^{+} - \rho_{w}^{-}\left(1 + \varepsilon_{V}^{-} \right)\varphi^{-} S_{lq}^{-} \\
m_{ad}^{+} &= m_{ad}^{-} + \rho_{ad}^{+}\left(1 + \varepsilon_{V}^{+} \right)\varphi^{+} S_{lq}^{+} - \rho_{ad}^{-}\left(1 + \varepsilon_{V}^{-} \right)\varphi^{-} S_{lq}^{-} \\
m_{as}^{+} &= m_{as}^{-} + \rho_{as}^{+}\left(1 + \varepsilon_{V}^{+} \right)\varphi^{+}\left(1 - S_{lq}^{+} \right) - \rho_{as}^{-}\left(1 + \varepsilon_{V}^{-} \right)\varphi^{-}\left(1 - S_{lq}^{-} \right) \\
m_{vp}^{+} &= m_{vp}^{-} + \rho_{vp}^{+}\left(1 + \varepsilon_{V}^{+} \right)\varphi^{+}\left(1 - S_{lq}^{+} \right) - \rho_{vp}^{-}\left(1 + \varepsilon_{V}^{-} \right)\varphi^{-}\left(1 - S_{lq}^{-} \right)
\end{aligned}
\qquad \text{éq 4.2.5-1}
$$

4.2.6 Calculation of the heat-storage capacity and Q' heat

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 39/62
Clé : R7.01.11   Révision :
3731397193c7

$$C_\sigma^{0^+} = (1 - \varphi^+) \rho_s C_\sigma^s + S_{lq}^+ \varphi^+ (\rho_w^+ C_w^p + \rho_{ad}^+ C_{ad}^p) + (1 - S_{lq}^+) \varphi^+ (\rho_{vp}^+ C_{vp}^p + \rho_{as}^+ C_{as}^p) \qquad \text{éq 4.2.6-1}$$

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

$$C_\varepsilon^{0+} = C_\sigma^{0+} - T^+ (\boldsymbol{C}_0 : \boldsymbol{\alpha}_0) : \boldsymbol{\alpha}_0 \qquad \text{éq 4.2.6-2}$$

Note:

In the isotropic case [éq 4.2.6-2] becomes:

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

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

$$Q'^+ = Q'^- + (\boldsymbol{C}_0 : \boldsymbol{\alpha}_0) : (\boldsymbol{\varepsilon}^+ - \boldsymbol{\varepsilon}^-) T^{1/2} + 3 \alpha_{lq}^{m^+} T^{1/2} (p_c^+ - p_c^-) - (3 \alpha_{gz}^{m^+} + 3 \alpha_{lq}^{m^+}) T^{1/2} (p_{gz}^+ - p_{gz}^-) + C_\varepsilon^{0^+} (T^+ - T^-)$$
$$\text{éq 4.2.6-3}$$

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

Note:

In the isotropic case [éq 4.2.6-3] becomes:

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

4.2.7   Calculation of the mechanical constraints

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

$$\sigma_p^+ = \sigma_p^- - \boldsymbol{B} (p_{gz}^+ - p_{gz}^-) + \boldsymbol{B} S_{lq}^+ (p_c^+ - p_c^-) \qquad \text{éq 4.2.7-1}$$

In the isotropic case one has $\boldsymbol{B} = b.\boldsymbol{1}$, $\sigma_p^+ = \sigma_p^+.\boldsymbol{1}$ and $\sigma_p^- = \sigma_p^-.\boldsymbol{1}$

4.2.8   Calculation of hydrous and thermal flows

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

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

The thermal tensor of diffusivity $\boldsymbol{\lambda}^{T^+} = \lambda_\varphi^T (\varphi^+). \lambda_S^T (S_{lq}^+). \boldsymbol{\lambda}_T^T (T^+) + \boldsymbol{\lambda}_{cte}^T$

Tensors of permeability and hydraulic conductivity:

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 40/62
Clé : R7.01.11   Révision   :
3731397193c7

In the isotropic case, $K^{int} = K^{int} \cdot \mathbf{1}$, $\boldsymbol{\lambda}^T = \lambda^T \cdot \mathbf{1}$, $\boldsymbol{\lambda}_T^T(T) = \lambda_T^T(T) \cdot \mathbf{1}$ and $\boldsymbol{\lambda}_{cte}^T = \lambda_{cte}^T \cdot \mathbf{1}$.

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

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

$$\frac{M_{as}^+}{\rho_{as}^+} = \boldsymbol{\lambda}_{gz}^{H^+} \left[-\nabla p_{gz}^+ + \left(\rho_{as}^+ + \rho_{vp}^+ \right) F^m \right] + C_{vp}^+ F_{vp}^+ \nabla C_{vp}^+ \qquad \text{éq 4.2.8-2}$$

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

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

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

In the isotropic cases, $\boldsymbol{\lambda}_{lq}^H = \lambda_{lq}^H \cdot \mathbf{1}$ and $\boldsymbol{\lambda}_{gz}^H = \lambda_{gz}^H \cdot \mathbf{1}$

5 Calculation of the derivative of the generalized constraints

In this chapter, we give the expressions of the derivative of the constraints generalized compared to the deformations generalized within the meaning of the document [R7.01.10] [4], i.e. the terms which are calculated when the laws of behaviors THM are called for the option RIGI_MECA_TANG within the meaning of the document [R5.03.01] [3].

In order not to weigh down the talk, we give the expression of the differentials of the generalized constraints, knowing that the derivative partial result some directly.

5.1 Derived from the constraints

The calculation of the differential of the effective constraints is left with the load of the purely mechanical law of behavior, which we do not describe in this document. Differential of the constraint σ_p is given directly by the expression [éq 3.2.8-2].

5.2 Derived from the mass contributions

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

Code_Aster

Version
default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 41/62
Clé : R7.01.11   *Révision   :*
                     3731397193c7

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

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

éq 5.2-1

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

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

5.2.1 Case without dissolved air

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:

$$\left.\begin{array}{l}\dfrac{dm_w}{\rho_w} = S_{lq}\,\boldsymbol{B}:\boldsymbol{d\,\varepsilon} + \left(\varphi\dfrac{\partial S_{lq}}{\partial P_c} - \dfrac{S_{lq}\varphi}{K_w} - \dfrac{S_{lq}^2}{M_\varphi}\right)dp_c + S_{lq}\left(\dfrac{\varphi}{K_w} + \dfrac{1}{M_\varphi}\right)dp_{gz} - 3\,\alpha_w^m\,dT \\[3mm] \dfrac{dm_{vp}}{\rho_{vp}} = \left(1-S_{lq}\right)\boldsymbol{B}:\boldsymbol{d\,\varepsilon} + \left(-\varphi\dfrac{\partial S_{lq}}{\partial P_c} - \dfrac{\left(1-S_{lq}\right)S_{lq}}{M_\varphi}\right)dp_c + \left(\dfrac{\left(1-S_{lq}\right)}{M_\varphi}\right)dp_{gz} + \varphi\left(1-S_{lq}\right)\dfrac{dp_{vp}}{p_{vp}} - 3\,\alpha_{vp}^m\,dT \\[3mm] \dfrac{dm_{as}}{\rho_{as}} = \left(1-S_{lq}\right)\boldsymbol{B}:\boldsymbol{d\,\varepsilon} + \left(-\varphi\dfrac{\partial S_{lq}}{\partial P_c} - \dfrac{\left(1-S_{lq}\right)S_{lq}}{M_\varphi}\right)dp_c + \left(\dfrac{\left(1-S_{lq}\right)}{M_\varphi}\right)dp_{gz} + \varphi\left(1-S_{lq}\right)\dfrac{dp_{as}}{p_{as}} - 3\,\alpha_{as}^m\,dT\end{array}\right\}$$

éq 5.2.1-1

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

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

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

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:

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 42/62
Clé : R7.01.11   Révision :
3731397193c7

$$\frac{dm_w}{\rho_w} = S_{lq} \boldsymbol{B} : \boldsymbol{d}\,\varepsilon + \left(\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{S_{lq}\varphi}{K_w} - \frac{S_{lq}^2}{M_\varphi} \right) dp_c + S_{lq}\left(\frac{\varphi}{K_w} + \frac{1}{M_\varphi} \right) dp_{gz} - 3\alpha_w^m dT \qquad \textbf{éq 5.2.1-3}$$

$$\frac{dm_{vp}}{\rho_{vp}} = (1 - S_{lq})\boldsymbol{B} : \boldsymbol{d}\,\varepsilon + \left(-\varphi \frac{\partial S_{lq}}{\partial p_c} - \frac{(1 - S_{lq})S_{lq}}{M_\varphi} - \frac{\varphi(1 - S_{lq})}{p_{vp}}\frac{\rho_{vp}}{\rho_{lq}} \right) dp_c$$

$$+ \left(\frac{(1 - S_{lq})}{M_\varphi} - \frac{\varphi(1 - S_{lq})}{p_{vp}}\frac{\rho_{vp}}{\rho_{lq}} \right) dp_{gz} \qquad\qquad \textbf{éq 5.2.1-4}$$

$$+ \left(-3\alpha_{vp}^m + \frac{\rho_{vp}\varphi(1 - S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{vp}T} \right) dT$$

$$\frac{dm_{as}}{\rho_{as}} = (1 - S_{lq})\boldsymbol{B} : \boldsymbol{d}\,\varepsilon + \left(-\varphi \frac{\partial S_{lq}}{\partial p_c} - \frac{(1 - S_{lq})S_{lq}}{M_\varphi} - \frac{\varphi(1 - S_{lq})}{p_{as}}\frac{\rho_{vp}}{\rho_{lq}} \right) dp_c$$

$$+ \left(\frac{(1 - S_{lq})}{M_\varphi} - \frac{\varphi(1 - S_{lq})}{p_{as}}\frac{\rho_{lq} - \rho_{vp}}{\rho_{lq}} \right) dp_{gz} + \left(-3\alpha_{as}^m + \frac{\rho_{vp}\varphi(1 - S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{as}T} \right) dT \qquad \textbf{éq 5.2.1-5}$$

5.2.2 Case with dissolved air

As 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:

$$\frac{dm_w}{\rho_w} = bS_{lq}\,d\,\varepsilon_V + \left(\frac{S_{lq}\varphi}{K_w}\frac{\partial p_w}{\partial P_c} - \frac{S_{lq^2}(b - \varphi)}{K_s} + \varphi \frac{\partial S_{lq}}{\partial P_c} \right) dp_c + S_{lq}\left(\frac{\varphi}{K_w}\frac{\partial p_w}{\partial P_{gz}} + \frac{(b - \varphi)}{K_s} \right) dp_{gz} +$$

$$\left(\frac{\varphi S_{lq}}{K_w}\frac{\partial p_w}{\partial T} - 3\alpha_w^m \right) dT \qquad\qquad \textbf{éq 5.2.2-1}$$

$$\frac{dm_{ad}}{\rho_{ad}} = bS_{lq}\,d\,\varepsilon_V + \left(\frac{S_{lq}\varphi M_{as}^{ol}}{\rho_{ad}K_H}\frac{\partial p_{as}}{\partial P_c} - \frac{S_{lq^2}(b - \varphi)}{K_s} + \varphi \frac{\partial S_{lq}}{\partial P_c} \right) dp_c +$$

$$S_{lq}\left(\frac{\varphi M_{as}^{ol}}{\rho_{ad}K_H}\frac{\partial p_{as}}{\partial P_{gz}} + \frac{(b - \varphi)}{K_s} \right) dp_{gz} + S_{lq}\left(\frac{\varphi M_{as}^{ol}}{\rho_{ad}K_H}\frac{\partial p_{as}}{\partial T} - 3\alpha_0(b - \varphi) \right) dT \qquad \textbf{éq 5.2.2-2}$$

$$\frac{dm_{vp}}{\rho_{vp}} = b(1 - S_{lq})\,d\,\varepsilon_V + \left(-\varphi \frac{\partial S_{lq}}{\partial P_c} - \frac{(1 - S_{lq})S_{lq}(b - \varphi)}{K_s} - \frac{\varphi(1 - S_{lq})}{p_{vp}}\frac{\rho_{vp}}{\rho_{lq}} \right) dp_c +$$

$$\left(\frac{(b - \varphi)(1 - S_{lq})}{K_s} + \frac{\varphi(1 - S_{lq})}{p_{vp}}\frac{\rho_{vp}}{\rho_{lq}} \right) dp_{gz} + \left(-3\alpha_{vp}^m + \frac{\varphi\rho_{vp}(1 - S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{vp}T} \right) dT \qquad \textbf{éq 5.2.2-3}$$

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 43/62
Clé : R7.01.11   Révision   :
3731397193c7

$$\frac{dm_{as}}{\rho_{as}} = b(1-S_{lq})d\,\varepsilon_V + \left(-\varphi\frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}(b-\varphi)}{K_s} + \frac{\varphi(1-S_{lq})}{p_{as}}\frac{\rho_{vp}}{\rho_{lq}}\right)dp_c +$$

$$\left(\frac{(b-\varphi)(1-S_{lq})}{K_s} + \frac{\varphi(1-S_{lq})}{p_{as}}\frac{\rho_{lq}-\rho_{vp}}{\rho_{lq}}\right)dp_{gz} + \left(-3\alpha_{vp}^m - \frac{\varphi\rho_{vp}(1-S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{as}T}\right)dT$$

éq 5.2.2-4

The derivative partial are given in [§ Annexe 3].

5.3   Derived from the enthali and Q' heat

There still, we do nothing but point out expressions already provided to chapter 2:

5.3.1   Case without dissolved air

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

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

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

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

5.3.2   Case with dissolved air

As 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:

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 44/62
Clé : R7.01.11   Révision :
3731397193c7

$$\frac{dm_w}{\rho_w} = S_{lq} \boldsymbol{B} : \boldsymbol{d\,\varepsilon} + \left(\frac{S_{lq}\,\varphi}{K_w}\frac{\partial p_w}{\partial P_c} - \frac{S_{lq}^2}{M_\varphi} + \varphi\frac{\partial S_{lq}}{\partial P_c}\right)dp_c + S_{lq}\left(\frac{\varphi}{K_w}\frac{\partial p_w}{\partial P_{gz}} + \frac{1}{M_\varphi}\right)dp_{gz} + \left(\frac{\varphi\,S_{lq}}{K_w}\frac{\partial p_w}{\partial T} - 3\alpha_w^m\right)dT$$

éq 5.2.2-1

$$\frac{dm_{ad}}{\rho_{ad}} = S_{lq}\boldsymbol{B}:\boldsymbol{d\,\varepsilon} + \left(\frac{S_{lq}\,\varphi\,M_{as}^{ol}}{\rho_{ad}K_H}\frac{\partial p_{as}}{\partial P_c} - \frac{S_{lq}^2}{M_\varphi} + \varphi\frac{\partial S_{lq}}{\partial P_c}\right)dp_c + S_{lq}\left(\frac{\varphi\,M_{as}^{ol}}{\rho_{ad}K_H}\frac{\partial p_{as}}{\partial P_{gz}} + \frac{1}{M_\varphi}\right)dp_{gz}$$
$$+ S_{lq}\left(\frac{\varphi\,M_{as}^{ol}}{\rho_{ad}K_H}\frac{\partial p_{as}}{\partial T} - 3\alpha_\varphi\right)dT$$

éq 5.2.2-2

$$\frac{dm_{vp}}{\rho_{vp}} = (1-S_{lq})\boldsymbol{B}:\boldsymbol{d\,\varepsilon} + \left(-\varphi\frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}}{M_\varphi} - \frac{\varphi(1-S_{lq})}{p_{vp}}\frac{\rho_{vp}}{\rho_{lq}}\right)dp_c + \left(\frac{(1-S_{lq})}{M_\varphi} + \frac{\varphi(1-S_{lq})}{p_{vp}}\frac{\rho_{vp}}{\rho_{lq}}\right)dp_{gz} +$$
$$+ \left(-3\alpha_{vp}^m + \frac{\varphi\,\rho_{vp}(1-S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{vp}T}\right)dT$$

éq 5.2.2-3

$$\frac{dm_{as}}{\rho_{as}} = (1-S_{lq})\boldsymbol{B}:\boldsymbol{d\,\varepsilon} + \left(-\varphi\frac{\partial S_{lq}}{\partial P_c} - \frac{(1-S_{lq})S_{lq}}{M_\varphi} + \frac{\varphi(1-S_{lq})}{p_{as}}\frac{\rho_{vp}}{\rho_{lq}}\right)dp_c +$$
$$\left(\frac{((1-S_{lq}))}{M_\varphi} + \frac{\varphi(1-S_{lq})}{p_{as}}\frac{\rho_{lq}-\rho_{vp}}{\rho_{lq}}\right)dp_{gz} + \left(-3\alpha_{vp}^m - \frac{\varphi\,\rho_{vp}(1-S_{lq})(h_{vp}^m - h_{lq}^m)}{p_{as}T}\right)dT$$

éq 5.2.2-4

The derivative partial are given in [§Annexe 3].

5.4 Derived from the enthali and Q' heat

There still, we do nothing but point out expressions already provided to chapter 2:

5.4.1 Case without dissolved air

$$dh_w^m = \left(1 - 3\alpha_w T\right)\frac{dp_{gz} - dp_c}{\rho_w} + C_w^p dT$$
$$dh_{vp}^m = C_{vp}^p dT$$
$$dh_{as}^m = C_{as}^p dT$$
$$\delta Q' = (\boldsymbol{C_0}:\boldsymbol{\alpha_0}:\boldsymbol{d\,\varepsilon})T + 3\alpha_{lq}^m Tdp_c - \left(3\alpha_{gz}^m + 3\alpha_{lq}^m\right)Tdp_{gz} + C_\varepsilon^0 dT$$

5.4.2 Case with dissolved air

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 45/62
Clé : R7.01.11   Révision   :
3731397193c7

$$dh_{ad}^m = C_{ad}^p dT$$
$$dh_{vp}^m = C_{vp}^p dT$$
$$dh_{as}^m = C_{as}^p dT$$
$$\delta Q' = (\boldsymbol{C_0}:\boldsymbol{\alpha_0}:\boldsymbol{d\,\varepsilon})T + 3\alpha_{lq}^m Tdp_c - \left(3\alpha_{gz}^m + 3\alpha_{lq}^m\right)Tdp_{gz} + C_\varepsilon^0 dT$$

5.5 Derived from the heat flow

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

While differentiating [éq 3.2.5.1 - 2] and while using [éq 3.2.1-1], one finds:

$$d\lambda^T = \lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T}).\boldsymbol{B}:\boldsymbol{d\,\varepsilon}$$
$$+\frac{1}{M_\varphi}\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T})dp_{gz}$$
$$+\left(\lambda_\varphi^T(\varphi).\lambda_S^{T\,\prime}(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T}).\frac{\partial S_{lq}}{\partial p_c} - S_{lq}\frac{1}{M_\varphi}\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T})\right)dp_c$$
$$+\left(\lambda_\varphi^T(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^{T\,\prime}}(\boldsymbol{T}) - 3\alpha_\varphi\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T})\right)dT$$

That is to say finally:

$$\boldsymbol{dq} = -\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T}).\boldsymbol{B}:\boldsymbol{d\,\varepsilon}.\boldsymbol{\nabla}T$$
$$-\frac{1}{M_\varphi}\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T}).\boldsymbol{\nabla}T\,dp_{gz}$$
$$-\left(\lambda_\varphi^T(\varphi).\lambda_S^{T\,\prime}(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T}).\frac{\partial S_{lq}}{\partial p_c} - S_{lq}\frac{1}{M_\varphi}\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T})\right).\boldsymbol{\nabla}T\,dp_c$$
$$-\left(\lambda_\varphi^T(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^{T\,\prime}}(\boldsymbol{T}) - 3\alpha_\varphi\lambda_\varphi^{T\,\prime}(\varphi).\lambda_S^T(S_{lq}).\boldsymbol{\lambda_T^T}(\boldsymbol{T})\right).\boldsymbol{\nabla}T\,dT$$

éq 5.4-1

5.6 Derived from hydrous flows

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.

5.6.1 Case without dissolved air

$$d\mathbf{M}_{as} = \left(\frac{\mathbf{M}_{as}}{\rho_{as}} + \rho_{as}\boldsymbol{\lambda_{gz}^H}.\boldsymbol{F^m}\right)d\rho_{as} + (\mathbf{M}_{as} - \rho_{as}C_{vp}F_{vp}\boldsymbol{\nabla}C_{vp}).[\boldsymbol{\lambda_{lq}^H}]^{-1}d\boldsymbol{\lambda_{gz}^H}$$
$$+\rho_{as}\boldsymbol{\lambda_{gz}^H}\left(-d\boldsymbol{\nabla}p_{gz} + d\rho_{vp}\boldsymbol{F^m}\right)$$
$$+\rho_{as}C_{vp}\left(\frac{\partial F_{vp}}{\partial T}dT + \frac{\partial F_{vp}}{\partial p_{gz}}p_{gz}\right)\boldsymbol{\nabla}C_{vp} + \rho_{as}dC_{vp}F_{vp}\boldsymbol{\nabla}C_{vp} + \rho_{as}C_{vp}F_{vp}d\boldsymbol{\nabla}C_{vp}$$

éq 5.5.1-1

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 46/62
Clé : R7.01.11   Révision   :
3731397193c7

$$d\,\mathbf{M}_{vp} = \left(\frac{\mathbf{M}_{vp}}{\rho_{vp}} + \rho_{vp}\boldsymbol{\lambda}_{gz}^{H}\cdot\boldsymbol{F}^{m}\right)d\,\rho_{vp} + \left(\mathbf{M}_{vp} + \rho_{vp}(1-C_{vp})F_{vp}\boldsymbol{\nabla}\,C_{vp}\right).\left[\boldsymbol{\lambda}_{gz}^{H}\right]^{-1}.d\,\boldsymbol{\lambda}_{gz}^{H}$$

$$+ \rho_{vp}\boldsymbol{\lambda}_{gz}^{H}\left(-d\,\boldsymbol{\nabla}\,p_{gz} + d\,\rho_{as}\boldsymbol{F}^{m}\right)$$

$$-(1-C_{vp})\rho_{vp}\left(\frac{\partial F_{vp}}{\partial T}dT + \frac{\partial F_{vp}}{\partial p_{gz}}p_{gz}\right)\boldsymbol{\nabla}\,C_{vp} + \rho_{vp}dC_{vp}F_{vp}\boldsymbol{\nabla}\,C_{vp} - \rho_{vp}(1-C_{vp})F_{vp}d\,\boldsymbol{\nabla}\,C_{vp}$$

éq 5.5.1-2

$$d\,\mathbf{M}_{w} = \left(\frac{\mathbf{M}_{w}}{\rho_{w}} + \rho_{w}\boldsymbol{\lambda}_{lq}^{H}\cdot\boldsymbol{F}^{m}\right)d\,\rho_{w} + \left[\boldsymbol{\lambda}_{lq}^{H}\right]^{-1}.\mathbf{M}_{w}.d\,\boldsymbol{\lambda}_{lq}^{H}$$

$$-\rho_{w}\boldsymbol{\lambda}_{lq}^{H}\left(d\,\boldsymbol{\nabla}\,p_{gz} - d\,\boldsymbol{\nabla}\,p_{c}\right)$$

éq 5.5.1-3

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

$$dp_{as} = dp_{gz} - dp_{vp} = \frac{\rho_{w} - \rho_{vp}}{\rho_{w}}dp_{gz} + \frac{\rho_{vp}}{\rho_{w}}dp_{c} - \rho_{vp}\left(h_{vp}^{m} - h_{w}^{m}\right)\frac{dT}{T}$$

éq 5.5.1-4

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

$$d\,\rho_{vp} = \frac{\rho_{vp}^{2}}{\rho_{w}\,p_{gz}}dp_{gz} - \frac{\rho_{vp}^{2}}{\rho_{w}\,p_{vp}}dp_{c} + \left(\frac{\rho_{vp}^{2}\left(h_{vp}^{m} - h_{w}^{m}\right)}{Tp_{vp}} - \frac{\rho_{vp}}{T}\right)dT$$

éq 5.5.1-5

$$d\,\rho_{as} = \frac{\rho_{as}}{p_{as}}\frac{\rho_{w} - \rho_{vp}}{\rho_{w}}dp_{gz} + \frac{\rho_{as}}{p_{as}}\frac{\rho_{vp}}{\rho_{w}}dp_{c} + \left(-\frac{\rho_{as}\rho_{vp}\left(h_{vp}^{m} - h_{w}^{m}\right)}{Tp_{as}} - \frac{\rho_{as}}{T}\right)dT$$

éq 5.5.1-6

[éq 3.2.6-4] allows to express the gradient of the steam pressure:

$$\boldsymbol{\nabla}\,p_{vp} = \frac{\rho_{vp}}{\rho_{lq}}\left(\boldsymbol{\nabla}\,p_{gz} - \boldsymbol{\nabla}\,p_{c}\right) + \rho_{vp}\left(h_{vp}^{m} - h_{lq}^{m}\right)\frac{\boldsymbol{\nabla}\,T}{T}$$

éq 5.5.1-7

While differentiating [éq 5.5.1-7] one finds:

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 47/62
Clé : R7.01.11   Révision   :
3731397193c7

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

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

éq 5.5.1-8

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

$$d \left(\rho_{vp} \left(\frac{h_{vp}^m - h_w^m}{T} \right) \right) \nabla T = \left(\frac{h_{vp}^m - h_w^m}{T} \right) \nabla T d \rho_{vp} + \frac{\rho_{vp}}{T} \nabla T \left(dh_{vp}^m - dh_w^m \right) - \rho_{vp} \left(h_{vp}^m - h_w^m \right) \nabla T \frac{dT}{T^2}$$ **éq 5.5.1-9**

Knowing the differentials of its gradient and steam pressure, the expressions of the differentials of C_{vp} and of 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].

5.6.2   Case with dissolved air

$$d \mathbf{M}_{as} = \left(\frac{\mathbf{M}_{as}}{\rho_{as}} + \rho_{as} \boldsymbol{\lambda}_{gz}^H . \mathbf{F}^m \right) d \rho_{as} + \left(\mathbf{M}_{as} - \rho_{as} C_{vp} F_{vp} \nabla C_{vp} \right) . [\boldsymbol{\lambda}_{gz}^H]^{-1} . d \boldsymbol{\lambda}_{gz}^H$$

$$+ \rho_{as} \boldsymbol{\lambda}_{gz}^H \left(-d \nabla p_{gz} + d \rho_{vp} \mathbf{F}^m \right)$$ **éq 5.5.2-1**

$$+ \rho_{as} C_{vp} \left(\frac{\partial F_{vp}}{\partial T} dT + \frac{\partial F_{vp}}{\partial p_{gz}} dp_{gz} \right) \nabla C_{vp} + \rho_{as} dC_{vp} F_{vp} \nabla C_{vp} + \rho_{as} C_{vp} F_{vp} d \nabla C_{vp}$$

$$d \mathbf{M}_{vp} = \left(\frac{\mathbf{M}_{vp}}{\rho_{vp}} + \rho_{vp} \boldsymbol{\lambda}_{gz}^H . \mathbf{F}^m \right) d \rho_{vp} + \left(\mathbf{M}_{vp} + \rho_{vp} (1 - C_{vp}) F_{vp} \nabla C_{vp} \right) . [\boldsymbol{\lambda}_{gz}^H]^{-1} . d \boldsymbol{\lambda}_{gz}^H$$

$$+ \rho_{vp} \boldsymbol{\lambda}_{gz}^H \left(-d \nabla p_{gz} + d \rho_{as} \mathbf{F}^m \right)$$ **éq 5.5.2-2**

$$- (1 - C_{vp}) \rho_{vp} \left(\frac{\partial F_{vp}}{\partial T} dT + \frac{\partial F_{vp}}{\partial p_{gz}} dp_{gz} \right) \nabla C_{vp} + \rho_{vp} dC_{vp} F_{vp} \nabla C_{vp} - \rho_{vp} (1 - C_{vp}) F_{vp} d \nabla C_{vp}$$

$$d \mathbf{M}_w = \left(\frac{\mathbf{M}_w}{\rho_w} + \rho_w \boldsymbol{\lambda}_{lq}^H . \mathbf{F}^m \right) d \rho_w + \mathbf{M}_w . [\boldsymbol{\lambda}_{lq}^H]^{-1} . d \boldsymbol{\lambda}_{lq}^H + \rho_w \boldsymbol{\lambda}_{lq}^H \left(-d \nabla p_{lq} + d \rho_{ad} \mathbf{F}^m \right)$$ **éq 5.5.2-3**

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 48/62
Clé : R7.01.11   Révision   :
3731397193c7

$$d\,\mathbf{M}_{ad} = \left(-\lambda_{lq}^{H} \cdot \nabla\, p_{lq} + \rho_{lq}\,\lambda_{lq}^{H} \cdot \mathbf{F}^{m}\right) d\,\rho_{ad} + \rho_{ad}\left(-\lambda_{lq}^{H} \cdot (\nabla\, p_{lq} + \rho_{lq}\,\mathbf{F}^{m})\right) . d\,\lambda_{lq}^{H}$$
$$+ \rho_{ad}\,\lambda_{lq}^{H} \cdot \left(-d\,\nabla\, p_{lq} + d\,\rho_{w}\,\mathbf{F}^{m}\right)$$
$$-\left(\frac{\partial F_{ad}}{\partial T} dT + \frac{\partial F_{ad}}{\partial p_{c}} dp_{c}\right)\nabla C_{ad} - F_{ad}\,d\,\nabla C_{ad}$$

éq 5.5.2-4

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

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

$$d\,\rho_{as} = \frac{\rho_{as}}{p_{as}}\left(\frac{\partial p_{as}}{\partial p_{c}} dp_{c} + \frac{\partial p_{as}}{\partial p_{gz}} dp_{gz}\right) + \left(\frac{\rho_{as}}{p_{as}}\frac{\partial p_{as}}{\partial T} - \frac{\rho_{as}}{T}\right) dT$$

éq 5.5.2-5

$$d\,\rho_{vp} = \frac{\rho_{vp}}{p_{vp}}\left(\frac{\partial p_{vp}}{\partial p_{c}} dp_{c} + \frac{\partial p_{vp}}{\partial p_{gz}} dp_{gz}\right) + \left(\frac{\rho_{vp}}{p_{vp}}\frac{\partial p_{vp}}{\partial T} - \frac{\rho_{vp}}{T}\right) dT$$

éq 5.5.2-6

By using the relation [éq 3.2.3.1 - 1], one obtains:

$$d\,\rho_{w} = \frac{\rho_{w}}{K_{w}}\left(\frac{\partial p_{w}}{\partial p_{c}} dp_{c} + \frac{\partial p_{w}}{\partial p_{gz}} dp_{gz}\right) + \left(\frac{\rho_{w}}{K_{w}}\frac{\partial p_{w}}{\partial T} - 3\,\rho_{w}\,\alpha_{w}\right) dT$$

éq 5.5.2-7

And like $d\,\rho_{ad} = \dfrac{M_{as}^{ol}}{K_{H}} dp_{as}$,

$$d\,\rho_{ad} = \frac{M_{as}^{ol}}{K_{H}}\left(\frac{\partial p_{as}}{\partial p_{c}} dp_{c} + \frac{\partial p_{as}}{\partial p_{gz}} dp_{gz} + \frac{\partial p_{as}}{\partial T} dT\right)$$

éq 5.5.2-8

As previously, the expressions are used

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

$$dC_{vp} = \frac{1}{p_{gz}}\left(\frac{\partial p_{vp}}{\partial p_{c}} dp_{c} + \frac{\partial p_{vp}}{\partial T} dT\right) + \left(\frac{1}{p_{gz}}\frac{\partial p_{vp}}{\partial p_{gz}} - \frac{p_{vp}}{p_{gz}^{2}}\right) dp_{gz}$$

éq 5.5.2-9

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

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 49/62
Clé : R7.01.11   Révision   :
3731397193c7

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

éq 5.5.2-10

with

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

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

$$d \nabla p_{vp} = d \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + d \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + d \frac{\partial p_{vp}}{\partial T} \nabla T + \frac{\partial p_{vp}}{\partial p_{gz}} d \nabla p_{gz} + \frac{\partial p_{vp}}{\partial p_c} d \nabla p_c + \frac{\partial p_{vp}}{\partial T} d \nabla T$$

$$= \left(\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial T} \nabla T \right) dp_c$$

$$+ \left(\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial T} \nabla T \right) dp_{gz}$$

$$+ \left(\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_{gz}} \nabla p_{gz} + \frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_c} \nabla p_c + \frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial T} \nabla T \right) dT$$

$$+ \frac{\partial p_{vp}}{\partial p_{gz}} d \nabla p_{gz} + \frac{\partial p_{vp}}{\partial p_c} d \nabla p_c + \frac{\partial p_{vp}}{\partial T} d \nabla T$$

éq 5.5.2-12

The derivative 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

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

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

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

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

with

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 50/62
Clé : R7.01.11   Révision   :
3731397193c7

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

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

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

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

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021   Page : 51/62
Clé : R7.01.11   Révision   :
3731397193c7

6   Bibliography

[1]   O. COUSSY: "Mechanical of the porous environments". Éditions TECHNIP.

[2]   C. CHAVANT, P. CHARLES, Th. DUFORESTEL, F. VOLDOIRE: "Thermo-hydro-mechanics of the porous environments unsaturated in *Code_Aster* ". Note HI-74/99/011/A.

[3]   "Quasi static nonlinear algorithm (operator STAT_NON_LINE) ". Document *Aster* [R5.03.01].

[4]   "Modelings THHM general information and algorithms". Document *Aster* [R7.01.10].

[5]   A. GIRAUD: "Adaptation to the nonlinear model poroelastic of Lassabatère-Coussy to modeling porous environment unsaturated". (ENSG).

[6]   J. WABINSKI, F. VOLDOIRE: Thermohydromécanique in saturated medium. Note EDF/DER HI/74/96/010, of September 1996.

[7]   T. LASSABATERE: "Hydraulic couplings in porous environment unsaturated with phase shift: application to the withdrawal of desiccation of the concrete". Thesis ENPC.

[8]   PH. MESTAT, MR. PRAT: "Works in interaction". Hermes.

[9]   J.F. THILUS et al.: "Poro-mechanics", Biot Conference 1998.

[10] A.W. BISHOP & G.E. BLIGHT: "Nap Aspects of Effective Stress in Saturated and Partly Saturated Soils", Geotechnics n° 3 vol. XIII, pp. 177-197. 1963.

[11] A. constituent GIRAUD "Relation between macroscopic and microscopic properties of in the ansiotropic box". ENSG

[12] R. GIOT, A. GIRAUD, T. GUILLON "Three-dimensional poromechanical back aalysis of the pulsate transverse test accounting for isotropy. "Geotechnica 2012 7:151-165 recorded

[13] L. DORMIEUX, E. MIDDLE-CLASS "Introduction to the micromechanics of the porous environments". Press of the National school of the Highways Departments, Paris, ISBN 2 85978 364.4 (2002)

[14] G. concrete EI TABBAL "Drying behavior of: Application to nuclear waste packages". Thesis University Paris-Is. (2020)

[15] R. Badmann, NR. Stockausen, M.J. Setzer. "The statistical thickness and the chemical potential of adsorbed toilets films". J. Colloid Interfaces Sci 82,534-543. 1981

[16] E. Barrett, L. Joyner, P. Halenda. "The determination of pore volume and area distributions in porous substances." . Computations from Nitrogen Isotherms. *1896*. 1951

[17] S. Brunauer, P.H. Emett, E. Teller. "Adsorption of gases in multimolecular layers." J. amndt Chem. Ploughshare 60,309-319 (1938)

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	Version initial
7.4	C.Chavant, S.Granet, EDF-R&D/AMA	
9.2	S.Granet	Law of Van Genuchten

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 52/62
Clé : R7.01.11 Révision :
3731397193c7

	EDF-R&D/AMA	
10.2	S. Meunier, EDF R & D /AMA	Saturated Hydraulic modeling
11.2	F.Voldoire EDF-R&D/AMA	Modifications of working of the equations, some corrections here or there.
12.1	S.Granet EDF-R&D/AMA	Introduction of the transverse isotropy

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 53/62
Clé : R7.01.11   Révision :
3731397193c7

Annexe 1Generalized constraints and internal variables

Constraints:

Number	Name of component Aster	Contents
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	SIPXX	$\sigma_{p_{xx}}$
8	SIPYY	$\sigma_{p_{yy}}$
9	SIPZZ	$\sigma_{p_{zz}}$
10	SIPXY	$\sigma_{p_{xy}}$
11	SIPXZ	$\sigma_{p_{xz}}$
12	SIPYZ	$\sigma_{p_{yz}}$
13	M11	m_w
14	FH11X	M_{w_x}
15	FH11Y	M_{w_y}
16	FH11Z	M_{w_z}
17	ENT11	h_w^m
18	M12	m_{vp}
19	FH12X	M_{vp_x}
20	FH12Y	M_{vp_y}
21	FH12Z	M_{vp_z}
22	ENT12	h_{vp}^m
23	M21	m_{as}
24	FH21X	M_{as_x}
25	FH21Y	M_{as_y}
26	FH21Z	M_{as_z}
27	ENT21	h_{as}^m
28	M22	m_{ad}
29	FH22X	M_{ad_x}
30	FH22Y	M_{ad_y}

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 54/62
Clé : R7.01.11   Révision :
3731397193c7

31	FH22Z	M_{ad_z}
32	ENT22	h_{ad}^m
33	QPRIM	Q'
34	FHTX	q_x
35	FHTY	q_y
36	FHTZ	q_z

In the case without mechanics, and for the laws of behaviors (LIQU_VAPE_GAZ, LIQU_VAPE, LIQU_AD_GAZ_VAPE and LIQU_AD_GAZ) the internal variables are:

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

In the case without mechanics, and for the laws of behaviors (LIQU_GAZ, LIQU_GAZ_ATM,) the internal variables are:

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

In the case without mechanics, and for the laws of behaviors (LIQU_SATU,) the internal variables are:

Number	Name component Aster	Contents
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 mechanics (V1 in the elastic case, V1 and following for plastic models). The number of the internal variables above will have to then be incremented of as much.

Annexe 2 Data material

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

A2.1   Keyword factor **THM_LIQU**

♦	RHO	ρ_{lq}^0
◊	UN_SUR_K	$\dfrac{1}{K_{lq}}$

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 55/62
Clé : R7.01.11   Révision   :
3731397193c7

◊	ALPHA	α_{lq}
◊	CP	C_{lq}^{p}
◊	VISC	$\mu_{lq}(T)$
◊	D_VISC_TEMP	$\dfrac{\partial \mu_{lq}}{\partial T}(T)$

A2.2   Keyword factor `THM_GAZ`

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

A2.3   Keyword factor `THM_VAPE_GAZ`

◊	MASS_MOL	M_{VP}^{ol}
◊	CP	C_{vp}^{p}
◊	VISC	$\mu_{vp}(T)$
◊	D_VISC_TEMP	$\dfrac{\partial \mu_{vp}}{\partial T}(T)$

A2.4   Keyword factor `THM_AIR_DISS`

◊	CP	C_{ad}^{p}
◊	COEF_HENRY	K_{H}

A2.5   Keyword factor `THM_INIT`

♦	TEMP	^{init}T
♦	PRE1	$^{init}P_{1}$
♦	PRE2	$^{init}P_{2}$
♦	PORO	φ^{0}
♦	NEAR_VAPE	P_{vp}^{0}

It is pointed out that, according to modeling, the two pressures and represent:

	LIQU_SATU	LIQU_VAPE	LIQU_GAZ_ATM	GAS	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}

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 56/62
Clé : R7.01.11   Révision :
3731397193c7

A2.6   Keyword factor `THM_DIFFU`

♦	`R_GAZ`	R
◊	`RHO`	r_0
◊	`CP`	C_σ^S
◊	`BIOT_COEF`	b
◊	`BIOT_L`	b_L
◊	`BIOT_N`	b_N
◊	`BIOT_T`	b_T (case 2D)
◊	`SATU_PRES`	$S_{lq}(p_c)$
◊	`D_SATU_PRES`	$\dfrac{\partial S_{lq}}{\partial p_c}(p_c)$
◊	`PESA_X`	$\mathbf{F}_x^m$
◊	`PESA_Y`	$\mathbf{F}_y^m$
◊	`PESA_Z`	$\mathbf{F}_z^m$
◊	`PERM_IN`	$K^{int}(\varphi)$
◊	`PERMIN_L`	$K_L^{int}(\varphi)$
◊	`PERMIN_N`	$K_N^{int}(\varphi)$
◊	`PERMIN_T`	$K_T^{int}(\varphi)$ (case 2D)
◊	`PERM_LIQU`	$K_{lq}^{rel}(S_{lq})$
◊	`D_PERM_LIQU_SATU`	$\dfrac{\partial k_{lq}^{rel}}{\partial S_{lq}}(S_{lq})$
◊	`PERM_GAZ`	$k_{gz}^{rel}(S_{lq}, p_{gz})$
◊	`D_PERM_SATU_GAZ`	$\dfrac{\partial k_{gz}^{rel}}{\partial S_{lq}}(S_{lq}, p_{gz})$
◊	`D_PERM_PRES_GAZ`	$\dfrac{\partial k_{gz}^{rel}}{\partial p_{gz}}(S_{lq}, p_{gz})$
◊	`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`	$\dfrac{\partial f_{vp}^T}{\partial T}(T)$
◊	`D_FV_PG`	$\dfrac{\partial f_{vp}^{gz}}{\partial P_{gz}}(P_{gz})$
◊	`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`	$\dfrac{\partial f_{vp}^T}{\partial T}(T)$

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version
default

Date : 04/11/2021 Page : 57/62
Clé : R7.01.11   Révision   :
3731397193c7

◊   LAMB_T $\lambda_T^T(T)$

◊   LAMB_T_L $\lambda_T^T(T)$ according to L

◊   LAMB_T_N $\lambda_T^T(T)$ according to NR

◊   LAMB_T_T $\lambda_T^T(T)$ according to T (2D)

◊   D_LB_T $\dfrac{\partial \lambda_T^T(T)}{\partial T}$

◊   D_LB_T_L $\dfrac{\partial \lambda_T^T(T)}{\partial T}$ according to L

◊   D_LB_T_N $\dfrac{\partial \lambda_T^T(T)}{\partial T}$ according to NR

◊   D_LB_T_T $\dfrac{\partial \lambda_T^T(T)}{\partial T}$ according to T

◊   LAMB_PHI $\lambda_\phi^T(\phi)$

◊   D_LB_PHI $\dfrac{\partial \lambda_\phi^T(\phi)}{\partial \phi}$

◊   LAMB_S $\lambda_S^T(S)$

◊   DLAMBS $\dfrac{\partial \lambda_S^T(S)}{\partial S}$

◊   LAMB_CT λ_{CT}^T
◊   LAMB_CL λ_{CT}^T according to L
◊   LAMB_CN λ_{CT}^T according to NR
◊   LAMB_CT λ_{CT}^T according to T

Note:

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

Annexe 3 Derived from the pressures according to the generalized deformations

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

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 58/62
Clé : R7.01.11   Révision   :
3731397193c7

$$\left\{ \begin{array}{l} dp_{vp}\left[\dfrac{RT}{K_H}-\dfrac{\rho_w}{\rho_{vp}}\right]=\left(-L\,\rho_w+p_{ad}\right)\dfrac{dT}{T}+\left(\dfrac{RT}{K_H}-1\right)dp_{gz}+dp_c \\[4mm] dp_w\left[\dfrac{\rho_{vp}}{\rho_w}\dfrac{RT}{K_H}-1\right]=\left(-LR\dfrac{\rho_{vp}}{K_H}+\dfrac{p_{ad}}{T}\right)dT+\left(\dfrac{RT}{K_H}-1\right)dp_{gz}+dp_c \end{array} \right.$$

One can thus write the derivative partial of water and the vapor according to the generalized deformations:

$$\frac{\partial p_w}{\partial T}=\frac{-LR\dfrac{\rho_{vp}}{K_H}+\dfrac{p_{ad}}{T}}{\dfrac{\rho_{vp}}{\rho_w}\dfrac{RT}{K_H}-1}\;;\quad \frac{\partial p_w}{\partial p_{gz}}=\frac{\dfrac{RT}{K_H}-1}{\dfrac{\rho_{vp}}{\rho_w}\dfrac{RT}{K_H}-1}\;;\quad \frac{\partial p_w}{\partial p_c}=\frac{1}{\dfrac{\rho_{vp}}{\rho_w}\dfrac{RT}{K_H}-1}$$

$$\frac{\partial p_{vp}}{\partial T}\frac{\left(-L\,\rho_w+p_{ad}\right)}{\dfrac{RT}{K_H}-\dfrac{\rho_w}{\rho_{vp}}}\cdot\frac{1}{T}\;;\quad \frac{\partial p_{vp}}{\partial p_{gz}}\frac{\dfrac{RT}{K_H}-1}{\dfrac{RT}{K_H}-\dfrac{\rho_w}{\rho_{vp}}}\;;\quad \frac{\partial p_{vp}}{\partial p_c}\frac{1}{\dfrac{RT}{K_H}-\dfrac{\rho_w}{\rho_{vp}}}$$

Relations $dp_{as}=dp_{gz}-dp_{vp}$ and $dp_{ad}=dp_{gz}-dp_c-dp_w$ allow 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

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

Code_Aster

Version default

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Date : 04/11/2021 Page : 59/62
Clé : R7.01.11   Révision   :
3731397193c7

Annexe 4   Derived seconds from air and steam pressures dissolved according to the generalized deformations

One calculates here the derivative partial of the second order of the steam pressure necessary to the section

[§5.5.2]. One will note thereafter:

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

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

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

Derived seconds from the steam pressure:

$$\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_{gz}} = \frac{A2}{A1^2} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_c} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_{gz}} = \frac{A2}{A1^2} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_{gz}} = \frac{R}{K_H A1} - \frac{1}{A1^2} \left(\frac{RT}{K_H} - 1 \right) \left(\frac{R}{K_H} - \frac{\rho_w}{\rho_{vp}} A4 \right)$$

$$\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial p_c} = -\frac{\rho_w}{\rho_{vp}} \frac{1}{A1^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_c} \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial p_c} = -\frac{\rho_w}{\rho_{vp}} \frac{1}{A1^2} \left(\frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} - \frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial p_c} = -\frac{1}{A1^2} \left(\frac{R}{K_H} - \frac{\rho_w}{\rho_{vp}} A4 \right)$$

$$\frac{\partial}{\partial p_c} \frac{\partial p_{vp}}{\partial T} = -\frac{1}{T} \frac{1}{A1^2} \left(A1 \left(1 - \frac{\partial p_w}{\partial p_c} (1 + L \frac{\rho_w}{K_W}) \right) + (p_{ad} - L\rho_w) \frac{\rho_w}{\rho_{vp}} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_c} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_c} \right) \right)$$

$$\frac{\partial}{\partial p_{gz}} \frac{\partial p_{vp}}{\partial T} = -\frac{1}{T} \frac{1}{A1^2} \left(A1 \left(1 - \frac{\partial p_w}{\partial p_{gz}} (1 + L \frac{\rho_w}{K_W}) \right) + (p_{ad} - L\rho_w) \frac{\rho_w}{\rho_{vp}} \left(\frac{1}{K_w} \frac{\partial p_w}{\partial p_{gz}} - \frac{1}{p_{vp}} \frac{\partial p_{vp}}{\partial p_{gz}} \right) \right)$$

$$\frac{\partial}{\partial T} \frac{\partial p_{vp}}{\partial T} = \frac{1}{T . A1} \left(\frac{\partial p_{ad}}{\partial T} - L \left(\frac{\rho_w}{K_W} \frac{\partial p_w}{\partial T} - 3\alpha_w \rho_w \right) \right) - \frac{1}{T^2 . A1^2} \left(\frac{RT}{K_H} - \frac{\rho_w}{\rho_{vp}} + T \left(\frac{R}{K_H} - \frac{\rho_w}{\rho_{vp}} A4 \right) \right) (p_{ad} - L\rho_w)$$

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 60/62
Clé : R7.01.11   Révision   :
3731397193c7

Derived seconds from the dissolved air pressure:

$$\frac{\partial}{\partial p_c}\frac{\partial p_{ad}}{\partial p_{gz}}=\frac{RT}{K_H}\frac{A2}{A1^2}\left(\frac{1}{p_{vp}}\frac{\partial p_{vp}}{\partial p_c}-\frac{1}{K_w}\frac{\partial p_w}{\partial p_c}\right)$$

$$\frac{\partial}{\partial p_{gz}}\frac{\partial p_{ad}}{\partial p_{gz}}=\frac{RT}{K_H}\frac{A2}{A1^2}\left(\frac{1}{p_{vp}}\frac{\partial p_{vp}}{\partial p_{gz}}-\frac{1}{K_w}\frac{\partial p_w}{\partial p_{gz}}\right)$$

$$\frac{\partial}{\partial T}\frac{\partial p_{ad}}{\partial p_{gz}}=-R_{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1}+\left(\frac{\rho_w}{\rho_{vp}}\right)^2\frac{R}{K_H}\frac{A2}{A1^2}\left(1+A3.T\right)$$

$$\frac{\partial}{\partial p_c}\frac{\partial p_{ad}}{\partial p_c}=\frac{RT}{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1^2}\left(\frac{1}{p_{vp}}\frac{\partial p_{vp}}{\partial p_c}-\frac{1}{K_w}\frac{\partial p_w}{\partial p_c}\right)$$

$$\frac{\partial}{\partial p_{gz}}\frac{\partial p_{ad}}{\partial p_c}=\frac{RT}{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1^2}\left(\frac{1}{p_{vp}}\frac{\partial p_{vp}}{\partial p_{gz}}-\frac{1}{K_w}\frac{\partial p_w}{\partial p_{gz}}\right)$$

$$\frac{\partial}{\partial T}\frac{\partial p_{ad}}{\partial p_c}=\frac{R}{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1^2}\left(1+A3.T\right)$$

$$\frac{\partial}{\partial p_c}\frac{\partial p_{ad}}{\partial T}=\frac{1}{A1}\frac{\rho_w}{\rho_{vp}}\left(\frac{LR}{K_H}\frac{\rho_{vp}}{p_{vp}}\frac{\partial p_{vp}}{\partial p_c}-\frac{1}{T}\frac{\partial p_{ad}}{\partial p_c}\right)-\frac{RT}{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1^2}\left(\frac{LR}{K_H}\rho_{vp}-\frac{p_{ad}}{T}\right).A3$$

$$\frac{\partial}{\partial p_{gz}}\frac{\partial p_{ad}}{\partial T}=\frac{1}{A1}\frac{\rho_w}{\rho_{vp}}\left(\frac{LR}{K_H}\frac{\rho_{vp}}{p_{vp}}\frac{\partial p_{vp}}{\partial p_{gz}}-\frac{1}{T}\frac{\partial p_{ad}}{\partial p_{gz}}\right)-\frac{RT}{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1^2}\left(\frac{LR}{K_H}\rho_{vp}-\frac{p_{ad}}{T}\right).A3$$

$$\frac{\partial}{\partial T}\frac{\partial p_{ad}}{\partial T}=\frac{1}{A1}\frac{\rho_w}{\rho_{vp}}\left(\frac{LR\rho_{vp}}{K_H}\left(\frac{1}{p_{vp}}\frac{\partial p_{vp}}{\partial T}-\frac{1}{T}\right)+\frac{p_{ad}}{T^2}-\frac{1}{T}\frac{\partial p_{ad}}{\partial T}\right)-\frac{RT}{K_H}\frac{\rho_w}{\rho_{vp}}\frac{1}{A1^2}\left(\frac{LR}{K_H}\rho_{vp}-\frac{p_{ad}}{T}\right).\left(A3+\frac{1}{T}\right)$$

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 61/62
Clé : R7.01.11 Révision : 3731397193c7

Annexe 5 Equivalence with formulations ANDRA

In order to be able to fit in the ALLIANCE platform, it is necessary to be coherent with the formulations posed by the ANDRA. 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 law of Henry
- Diffusion in the liquid
- Diffusion in gas

Notice concerning the enthali:

It is required to have coherence between the two models that 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	$=\dfrac{\phi_w}{\rho_w S_w n}$
h_{vp}^m	$=\dfrac{\phi_v}{\rho_v(1-S_w)n}$
h_{as}^m	$=\dfrac{\phi_{as}}{\rho_{as}(1-S_w)n}$
$\mathbf{M}_{lq}$	$=\rho_w f_w$
$\mathbf{M}_{as}$	$=\rho_{as} f_{as}$
$\mathbf{M}_{vp}$	$=\rho_v f_v$

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

$$\frac{d\phi}{dt}+Div\left(\phi_w\frac{f_w}{S_w n}+\phi_{as}\frac{f_{as}}{(1-S_w)n}+\phi_v\frac{f_v}{(1-S_w)n}\right)+Div(q)-(T-T^0)\frac{d}{dt}\left[(1-n)\rho_s C_s\right]$$

$$+3\alpha_0 K_0 T\frac{d\varepsilon_v}{dt}+3\alpha_{lq}^m T\frac{dp_c}{dt}-3\left(\alpha_{lq}^m+\alpha_{gz}^m\right)T\frac{dp_{gz}}{dt}-9TK_0\alpha_{0^2}\frac{dT}{dt}$$

$$=\left(\rho_w f_w+\rho_v f_v+\rho_{as}f_{as}\right)g+\Theta$$

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

A5.2   Law of Henry

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

Code_Aster

Titre : Modèles de comportement THHM
Responsable : GRANET Sylvie

Version default

Date : 04/11/2021 Page : 62/62
Clé : R7.01.11   Révision   :
3731397193c7

In the formulation of *Code_Aster*, it is pointed out that the law of Henry is expressed in the form:

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

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 flow in the air according to the steam concentration d' in the air or the relative humidity is noted:

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

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

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

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

like the report of the pressures such as: $C_{vp} = \dfrac{p_{vp}}{p_{gz}}$.

The law of perfect gases makes it possible to write that $C_{vp} = \omega_g^e$ thus $\nabla \omega_g^e = \nabla C_{vp}$ and
$f_{Diff_v} = D_v . \nabla C_{vp}$.
Thus equivalence *Code_Aster*/ANDRA is written simply:

$$F_{vp} = D_v .$$

A5.4   Diffusion of the air dissolved in water

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

$$f_{a_{ds_z}} = D_a . \nabla \omega_l^a$$

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

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

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

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

$$F_{ad} = D_a .$$