

## Note of use of model THM

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### Summary:

Modelings THM exclusively treat evolution of the behaviors Thermo-Hydro-Mechanics of the saturated porous environments, or not, by one or two fluids. The digital and physical description as of these modelings in Code\_Aster is detailed in [R7.01.10] and [R7.01.11].

One details in this documentation the procedure to be followed to carry out simulations in the context of modelings THM. One describes in the first part the various stages of calculations within the framework general of continuous the mediums known as "generalized" (cf [R7.01.10]). In this part, one will not detail what relates to the mechanical models described elsewhere. One restricts in the second part the application of these modelings to treat the porous environments which undergo a degradation of their mechanical properties per damage of the ground or the rocks for example. For that, one extends modelings THM to the mediums with microstructure by taking of account the effects second gradient (cf [R5.04.03]). The objective is to correct the dependence with the space discretization of the solutions when the mechanical law of behavior considered is of lenitive type – what is the case for any fragile material, and thus the grounds in particular.

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## 1 Broad outlines

### 1.1 Context of studies THM

First of all, it is advisable to define the quite precise framework of calculations Thermo-Hydro-Mechanics. Those have as an exclusive application the study of the porous environments. Knowing that, modeling THM covers the mechanical evolution of these mediums and the flows in their centre. The latter relate to one or two fluids and are governed by the laws of Darcy (fluid darcéens). The problem of complete THM thus treats flow of or fluid (S), mechanics of the skeleton, as well as thermics: the resolution is very often entirely coupled. It can also be chained whenever the phenomena hydraulics and mechanics are slightly coupled.

**Note:**

In the expression of the laws of Darcy which is retained here, 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.

### 1.2 General information

Calculations are based on families of laws of behavior THM for the saturated and unsaturated porous environments. 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. The formulation of modeling Thermo-hydro-mechanics (THM) in porous environment such as it is made in *Code\_Aster* is detailed in [R7.01.11] and [R7.01.10]. All the notations employed here thus refer to it. One points out some essential notations however thereafter:

Concerning the fluids, one considers (the most complete case) two phases (liquid and gas) and two components called by convenience water and air. The following indices then 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:  $p_w(x, t)$ ,  $p_{ad}(x, t)$ ,  $p_{vp}(x, t)$ ,  $p_{as}(x, t)$ ,
- the temperature of the medium  $T(x, t)$ .

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 varies according to the laws of behaviors.

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  $p_{gz}(x, t) = p_{vp} + p_{as}$ ,
- capillary pressure  $p_c(x, t) = p_{gz} - p_{lq} = p_{gz} - p_w - p_{ad}$ .

We will see thereafter the terminology Aster for these variables.

## 1.3 Stages of calculations

For the stages necessary to the implementation of a calculation Aster, independently of aspects purely THM, one will refer to the documentation of each order used.

In any calculation Aster, several key stages must be carried out:

- Choice of modeling
- Data materials
- Initialization
- Calculation
- Postprocessing

These points are detailed in the following chapter.

## 2 Various stages of a calculation THM

### 2.1 Choice of the model

The digital processing in THM requires a quadratic grid since the elements are of type *P2* in displacement and *PI* in pressure and temperature in order to avoid problems of oscillations.

The choice is done by the use of the order `AFFE_MODELE` as in example Ci - below:

```
MODELE=AFFE_MODELE (MAILLAGE=MAIL,  
                    AFFE=_F (TOUT=' OUI ',  
                             PHENOMENE=' MECANIQUE ',  
                             MODELISATION=' AXIS_THH2MD',),),)
```

In all the cases, the phenomenon is 'MECHANICAL' (even if modeling does not contain mechanics). The user must then inform in an obligatory way the keyword `MODELING`. This keyword makes it possible to define the type of affected element in a kind of mesh. Modelings available in THM are indicated in the table 2.1-1.

#### Notice concerning the digital processing (keyword ending in D or S):

Modelings ending in the letter D indicate that one makes a treatment allowing of diagonaliser ("lumper") the matrix in order to avoid the oscillations for the hydraulic problems. For that the points of integration are taken at the tops of the elements. This treatment being adapted little to mechanics, one also has a modeling known as "selective". In this case, the capacitive terms are integrated into the tops whereas the diffusive terms are integrated into the points of Gauss. These modelings end in S. other modelings integrate all into the point of Gauss.

One highly advises with the user to use modelings D or S in the cases without mechanics and to use modeling S and for modelings with mechanics.

"Classical" modelings (without D nor S) are brought to be reabsorbed and are disadvised.

MODELING	Geometrical modeling	Phenomena taken into account
D_PLAN_HM	plane	Mechanics, hydraulics with an unknown pressure
D_PLAN_HMD	plane	Mechanics, hydraulics with an unknown pressure (lumpé)
D_PLAN_HMS	plane	Mechanics, hydraulics with an unknown pressure (selective)
D_PLAN_HM_SI	plane	Mechanics, hydraulics with an unknown pressure (under-integrated)
D_PLAN_HHM	plane	Mechanics, hydraulics with two unknown pressures
D_PLAN_HHMD	plane	Mechanics, hydraulics with two unknown pressures (lumpé)
D_PLAN_HHMS	plane	Mechanics, hydraulics with two unknown pressures (selective)
D_PLAN_HH2MD	plane	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
D_PLAN_HH2MS	plane	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (selective)
D_PLAN_HH2M_SI	plane	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (under-integrated). Only modeling validates in dynamics.
D_PLAN_THHD	plane	Thermics, hydraulics with two unknown pressures (lumpé)
D_PLAN_THH2D	plane	Thermics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
D_PLAN_THH2S	plane	Thermics, hydraulics with two unknown pressures and two components in the gas phase (selective)
D_PLAN_THM	plane	Thermics, mechanics, hydraulics with an unknown pressure
D_PLAN_THVD	plane	Thermics, mechanics, hydraulics with two unknown pressures (2 phases: liquid water and vapor) (lumpé)
D_PLAN_THMD	plane	Thermics, mechanics, hydraulics with an unknown pressure (lumpé)
D_PLAN_THMS	plane	Thermics, mechanics, hydraulics with an unknown pressure (selective)
D_PLAN_THHMD	plane	Thermics, mechanics, hydraulics with two unknown pressures (lumpé)
D_PLAN_THHMS	plane	Thermics, mechanics, hydraulics with two unknown pressures (selective)
D_PLAN_HHD	plane	hydraulics with two unknown pressures (lumpé)
D_PLAN_HHS	plane	hydraulics with two unknown pressures (selective)
D_PLAN_HH2D	plane	hydraulics with two unknown pressures and two components in the gas phase (lumpé)
D_PLAN_HH2S	plane	hydraulics with two unknown pressures and two components in the gas phase (selective)
D_PLAN_THH2MD	plan	Thermics, mechanics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
D_PLAN_THH2MS	plane	Thermics, mechanics, hydraulics with two unknown pressures and two components in the gas phase (selective)
AXIS_HM	axisymmetric	Mechanics, hydraulics with an unknown pressure
AXIS_HMD	axisymmetric	Mechanics, hydraulics with an unknown pressure (lumpé)
AXIS_HMS	axisymmetric	Mechanics, hydraulics with an unknown pressure (selective)
AXIS_HHM	axisymmetric	Mechanics, hydraulics with two unknown pressures
AXIS_HHMD	axisymmetric	Mechanics, hydraulics with two unknown pressures (lumpé)
AXIS_HHMS	axisymmetric	Mechanics, hydraulics with two unknown pressures (selective)
AXIS_HH2MD	axisymmetric	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
AXIS_HH2MS	axisymmetric	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (selective)
AXIS_THHD	axisymmetric	Thermics, hydraulics with two unknown pressures (lumpé)
AXIS_THHS	axisymmetric	Thermics, hydraulics with two unknown pressures (selective)
AXIS_THH2D	axisymmetric	Thermics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)

MODELING	Geometrical modeling	Phenomena taken into account
AXIS_THH2S	axisymmetric	Thermics, hydraulics with two unknown pressures and two components in the gas phase (selective)
AXIS_THM	axisymmetric	Thermics, mechanics, hydraulics with an unknown pressure
AXIS_THMD	axisymmetric	Thermics, mechanics, hydraulics with an unknown pressure (lumpé)
AXIS_THMS	axisymmetric	Thermics, mechanics, hydraulics with an unknown pressure (selective)
AXIS_THVD	axisymmetric	Thermics, mechanics, hydraulics with two unknown pressures (2 phases: liquid water and vapor) (lumpé)
AXIS_THHMD	axisymmetric	Thermics, mechanics, hydraulics with two unknown pressures (lumpé)
AXIS_THHMS	axisymmetric	Thermics, mechanics, hydraulics with two unknown pressures (selective)
AXIS_THH2MD	axisymmetric	Thermics, mechanics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
AXIS_THH2MS	axisymmetric	Thermics, mechanics, hydraulics with two unknown pressures and two components in the gas phase (selective)
AXIS_HHD	axisymmetric	hydraulics with two unknown pressures (lumpé)
AXIS_HHS	axisymmetric	hydraulics with two unknown pressures (selective)
AXIS_HH2D	axisymmetric	hydraulics with two unknown pressures and two components in the gas phase (lumpé)
AXIS_HH2S	axisymmetric	hydraulics with two unknown pressures and two components in the gas phase (selective)
3D_HM	3D	Mechanics, hydraulics with an unknown pressure
3D_HMD	3D	Mechanics, hydraulics with an unknown pressure (lumpé)
3D_HMS	3D	Mechanics, hydraulics with an unknown pressure (selective)
3D_HM_SI	3D	Mechanics, hydraulics with an unknown pressure (under-integrated)
3D_HHM	3D	Mechanics, hydraulics with two unknown pressures
3D_HHMD	3D	Mechanics, hydraulics with two unknown pressures (lumpé)
3D_HHMS	3D	Mechanics, hydraulics with two unknown pressures (selective)
3D_HH2MD	3D	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
3D_HH2MS	3D	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (selective)
3D_HH2M_SI	3D	Mechanics, hydraulics with two unknown pressures and two components in the gas phase (under-integrated). Only modeling validates in dynamics.
3D_THHD	3D	Thermics, hydraulics with two unknown pressures (lumpé)
3D_THH2D	3D	Thermics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
3D_THH2S	3D	Thermics, hydraulics with two unknown pressures and two components in the gas phase (selective)
3D_THM	3D	Thermics, mechanics, hydraulics with an unknown pressure
3D_THMD	3D	Thermics, mechanics, hydraulics with an unknown pressure (lumpé)
3D_THMS	3D	Thermics, mechanics, hydraulics with an unknown pressure (selective)
3D_THVD	3D	Thermics, mechanics, hydraulics with two unknown pressures (2 phases: liquid water and vapor) (lumpé)
3D_THHM	3D	Thermics, mechanics, hydraulics with two unknown pressures
3D_THHMD	3D	Thermics, mechanics, hydraulics with two unknown pressures (lumpé)
3D_THHMS	3D	Thermics, mechanics, hydraulics with two unknown pressures (selective)

MODELING	Geometrical modeling	Phenomena taken into account
3D_THH2MD	3D	Thermics, mechanics, hydraulics with two unknown pressures and two components in the gas phase (lumpé)
3D_THH2MS	3D	Thermics, mechanics, hydraulics with two unknown pressures and two components in the gas phase (selective)
3D_HHD	3D	hydraulics with two unknown pressures (lumpé)
3D_HHS	3D	hydraulics with two unknown pressures (selective)
3D_HH2D	3D	hydraulics with two unknown pressures and two components in the gas phase (lumpé)
3D_HH2S	3D	hydraulics with two unknown pressures and two components in the gas phase (selective)

Table 2.1-1: Modelings THM

The principal unknown factors which are also the values of the degrees of freedom, are noted in the case of the most complete modeling (thermal, mechanical, hydraulic 3D with two unknown pressures).

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

Contents of *PRE1* and *PRE2* depends on the selected coupling and will be clarified in the section 2.2.2.

According to modeling chosen, only some of these degrees of freedom exist. The table above summarizes the degrees of freedom used for each modeling.

MODELING	$u_x$	$u_y$	$u_z$	<i>PRE1</i> <sup>ddl</sup>	<i>PRE2</i> <sup>ddl</sup>	<i>T</i> <sup>ddl</sup>
D PLAN HM ( , S, D, IF)	X	X		X		
D PLAN HHM ( , S, D)	X	X		X	X	
D PLAN HH2M (S, D, SI)	X	X		X	X	
D PLAN THH (S, D)				X	X	X
D PLAN THH2 (S, D)				X	X	X
D PLAN THM ( , S, D)	X	X		X		X
D PLAN THV ( , S, D)				X	X	X
D PLAN THHM (S, D)	X	X		X	X	X
D PLAN THH2M (S, D)	X	X		X	X	X
D PLAN HH (S, D)				X	X	
D PLAN HH2 (S, D)				X	X	
AXIS HM ( , S, D)	X	X		X		
AXIS HHM ( , S, D)	X	X		X	X	
AXIS HH2M (S, D)	X	X		X	X	
AXIS THH (S, D)				X	X	X
AXIS THH2 (S, D)				X	X	X
AXIS THM ( , S, D)	X	X		X		X
AXIS THV ( , S, D)				X	X	X
AXIS THHM (S, D)	X	X		X	X	X
AXIS THH2M (S, D)	X	X		X	X	X
AXIS HH (S, D)				X	X	
AXIS HH2 (S, D)				X	X	



MODELING	$u_x$	$u_y$	$u_z$	$PRE1^{ddl}$	$PRE2^{ddl}$	$T^{ddl}$
3D HM( , S, D, IF)	X	X	X	X		
3D HHM( , S, D)	X	X	X	X	X	
3D HH2M(S, D, _SI)	X	X	X	X	X	
3D THH(S, D)				X	X	X
3D THH2D				X	X	X
3D THM( , S, D)	X	X	X	X		X
3D THVD( , S, D)				X	X	X
3D THHM( , S, D)	X	X	X	X	X	X
3D THH2M(S, D)	X	X	X	X	X	X
3D HH(S, D)				X	X	
3D HH2(S, D)				X	X	

The generalized constraints and the internal variables all are indicated in [§Annexe 1]. The notations used are those defined in [R7.01.11].

## 2.2 Definition of material

The material is defined by the order `DEFI_MATERIAU` as in example Ci - below:

```
MATERBO=DEFI_MATERIAU (ELAS=_F (E=5.15000000E8,
                                NU=0.20,
                                ALPHA=0.),),
COMP_THM = 'LIQU_AD_GAZ_VAPE',
THM_LIQU=_F (RHO=1000.0,
             UN_SUR_K=0.,
             ALPHA=0.,
             CP=0.0,
             VISC=VISCOLIQ,
             D_VISC_TEMP=DVISCOL,),
THM_GAZ=_F (MASS_MOL=0.01,
            CP=0.0,
            VISC=VISCOGAZ,
            D_VISC_TEMP=ZERO,),
THM_VAPE_GAZ=_F (MASS_MOL=0.01,
                 CP=0.0,
                 VISC=VISCOGAZ,
                 D_VISC_TEMP=ZERO,),
THM_AIR DISS=_F (
                 CP=0.0,
                 COEF_HENRY=HENRY
                 ),
THM_INIT=_F (TEMP=300.0,
             PRE1=0.0,
             PRE2=1.E5,
             PORO=1.,
             PRES_VAPE=1000.0,
             ),
THM_DIFFU=_F (R_GAZ=8.32,
              RHO=2200.0,
              CP=1000.0,
              BIOT_COEF=1.0,
              SATU_PRES=SATUBO,
              D_SATU_PRES=DSATBO,
              PESA_X=0.0,
              PESA_Y=0.0,
              PESA_Z=0.0,
              PERM_IN=KINTBO,
              PERM_LIQU=UNDEMI,
```

```
D_PERM_LIQU_SATU=ZERO,  
PERM_GAZ=UNDEMI,  
D_PERM_SATU_GAZ=ZERO,  
D_PERM_PRES_GAZ=ZERO,  
FICKV_T=ZERO,  
FICKA_T=FICK,  
LAMB_T=ZERO,  
,,);
```

We now will detail each keywords. We will not stick here to the mechanical part – so mechanical there is - which depends on the selected law of behavior. One will refer for that to the documentation of `DEFI_MATERIAU` (U4.43.01).

## 2.2.1 Simple keyword `COMP_THM`

Allows to select as of the definition of material the mixing rate THM. The possible laws are

```
◆ COMP_THM = / 'LIQU_SATU ' ,  
              / 'LIQU_GAZ ' ,  
              / 'GAS ' ,  
              / 'LIQU_GAZ_ATM ' ,  
              / 'LIQU_AD_GAZ ' ,  
              / 'LIQU_VAPE_GAZ ' ,  
              / 'LIQU_AD_GAZ_VAPE ' ,  
              / 'LIQU_VAPE ' ,  
/ 'GAS'
```

Law of reaction of a perfect gas i.e. checking the relation  $P/\rho = RT/M_V$  where  $P$  is the pressure,  $\rho$  density,  $M_V$  molar mass,  $R$  the constant of perfect gases and  $T$  the temperature (confer [R7.01.11] for more details). For an only saturated medium. The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keyword `THM_GAZ`.

```
/ 'LIQU_SATU'
```

Law of behavior for porous environments saturated by only one liquid (cf [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keyword `THM_LIQU`.

```
/ 'LIQU_GAZ_ATM'
```

Law of behavior for a porous environment unsaturated with a liquid and gas with atmospheric pressure (confer [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keywords `THM_LIQU` and `THM_GAZ`.

```
/ 'LIQU_VAPE_GAZ'
```

Law of behavior for a porous environment unsaturated water/vapor/dry air with phase shift (confer [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keywords `THM_LIQU`, `THM_VAPE` and `THM_GAZ`.

```
/ 'LIQU_AD_GAZ_VAPE'
```

Law of behavior for a porous environment unsaturated water/vapor/dry air/air dissolved with phase shift (confer [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keywords `THM_LIQU`, `THM_VAPE`, `THM_GAZ` and `THM_AIR DISS`.

```
/ 'LIQU_AD_GAZ'
```

Law of behavior for a porous environment unsaturated water/dry air/air dissolved with phase shift (confer [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keywords `THM_LIQU`, `THM_GAZ` and `THM_AIR DISS`.

/ `LIQU\_VAPE`

Law of behavior for porous environments saturated by a component present in liquid form or vapor with phase shift (confer [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keywords `THM_LIQU` and `THM_VAPE`. **This law is valid only for modelings of the type THVD.**

/ `LIQU\_GAZ`

Law of behavior for a porous environment unsaturated liquid/gas without phase shift (confer [R7.01.11] for more details). The data necessary of the field material are provided in the operator `DEFI_MATERIAU`, under the keywords `THM_LIQU` and `THM_GAZ`.

The table below summarizes the obligatory keywords for under orders clarified in the following sections according to the selected mixing rate.

- Legends:
- O Obligatory keyword
  - T Obligatory keyword in Thermics
  - Useless keyword for this kind of mixing rate
  - F Useful for the law but optional (definite by default)

	LIQU_SAT U	LIQU_GA Z	GAS	LIQU_GAZ_A TM	LIQU_VAPE_G AZ	LIQU_AD_G AZ_VAPE	LIQU_AD _GAZ	LIQU_VAPE
<b>THM_INIT</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>
PRE1	O	O	O	O	O	O	O	O
PRE2		O			O	O	O	
PORO	O	O	O	O	O	O	O	O
TEMP	T	T	T	T	O	O	O	O
PRES_VAPE					O	O	O	O
<b>THM_DIFFU</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>	<b>O</b>
R_GAZ		O	O		O	O	O	O
RHO	O	O	O	O	O	O	O	O
BIOT_COEF	O	O	O	O	O	O	O	O
PESA_X	O	O	O	O	O	O	O	O
PESA_Y	O	O	O	O	O	O	O	O
PESA_Z	O	O	O	O	O	O	O	O
<i>If law HYDR_UTIL (cf chapter 2.5) :</i>								
SATU_PRES				O	O	O	O	O
D_SATU_PRES				O	O	O	O	O
PERM_LIQU				O	O	O	O	O
D_PERM_LIQU_SA TU				O	O	O	O	O
PERM_GAZ					O	O	O	O
D_PERM_SATU_G AZ					O	O	O	O
D_PERM_PRES_G AZ					O	O	O	O
<i>If law HYDR_VGM or HYDR_VGC (cf chapter 2.5) :</i>								
VG_N					O	O	O	
VG_PR					O	O	O	
VG_SR					O	O	O	
VG_SMAX					O	O	O	
VG_SATUR					O	O	O	
FICKV_T					O	O		
FICKV_PV					F	F		
FICKV_PG					F	F		
FICKV_S					F	F		
D_FV_T					F	F		
D_FV_PG					F	F		
FICKA_T					O	O	O	
FICKA_PA					F	F	F	
FICKA_PL					F	F	F	
FICKA_S					F	F	F	
D_FA_T					F	F	F	
CP	T	T	T	T	T	T	T	T
PERM_IN/PERM_E ND/PERM_L, PERM_N, PERM_T	O	O	O	O	O	O	O	O
LAMB_T/LAMB_TL, LAMB_TN, LAMB_TT	T	T	T	T	T	T	T	T
LAMB_S								
LAMB_PHI								

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

LAMB_CT/LAMB_C								
L, LAMB_C_N,								
LAMB_C T								
D_LB_T/D_LB_TOU								
T, D_LB_TL,								
D_LB T,								
D_LB S								
D_LB PHI								
<b>THM LIQU</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
RHO	0	0	0	0	0	0	0	0
UN_SUR K	0	0	0	0	0	0	0	0
VISC	0	0	0	0	0	0	0	0
D_VISC_TEMP	0	0	0	0	0	0	0	0
ALPHA	T	T	T	T	T	T	T	T
CP	T	T	T	T	T	T	T	T
<b>THM GAZ</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
MASS_MOL	0	0	0	0	0	0	0	0
VISC	0	0	0	0	0	0	0	0
D_VISC_TEMP	0	0	0	0	0	0	0	0
CP	T	T	T	T	T	T	T	T
<b>THM VAPE_GAZ</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
MASS_MOL	0	0	0	0	0	0	0	0
CP	0	0	0	0	0	0	0	0
VISC	0	0	0	0	0	0	0	0
D_VISC_TEMP	0	0	0	0	0	0	0	0
<b>THM AIR DISS</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
CP	0	0	0	0	0	0	0	0
COEF_HENRY	0	0	0	0	0	0	0	0

The table below summarizes compatibility between the laws of behavior and modelings choisies:

MODELING	Hydraulic law of behavior authorized
*_HM (_, S, D, IF)	'LIQU_SATU', 'GAS', 'LIQU_GAZ ATM'
*_HHM (_, S, D)	'LIQU_GAZ', 'LIQU_VAPE_GAZ'
*_HH2M (S, D, _SI)	'LIQU_AD_GAZ', 'LIQU_AD_GAZ_VAPE'
*_THH (S, D)	'LIQU_GAZ', 'LIQU_VAPE_GAZ'
*_THH2 (S, D)	'LIQU_AD_GAZ', 'LIQU_AD_GAZ_VAPE'
*_THM (_, S, D)	'LIQU_SATU', 'GAS', 'LIQU_GAZ ATM'
*_THV (_, S, D)	'LIQU_VAPE'
*_THHM (S, D)	'LIQU_GAZ', 'LIQU_VAPE_GAZ'
*_THH2M (S, D)	'LIQU_AD_GAZ', 'LIQU_AD_GAZ_VAPE'
*_HH (S, D)	'LIQU_GAZ', 'LIQU_VAPE_GAZ'
*_HH2 (S, D)	'LIQU_AD_GAZ', 'LIQU_AD_GAZ_VAPE'

## 2.2.2 Keyword factor THM\_INIT

For all the behaviors Thermo-Hydro-Mechanics, it makes it possible to describe a state of reference of the structure (cf [R7.01.10] and [R7.01.11]). Its syntax is the following one:

```
THM_INIT = _F (
    ◇ TEMP      = temp ,      [R]
    ◆ PRE1      = pre1 ,      [R]
    ◇ PRE2      = pre2 ,      [R]
    ◆ PORO      = poro ,      [R]
    ◇ PRES_VAPE = pvap ,      [R]
```

For understanding these data well, it is necessary to distinguish the unknown factors with the nodes, which we call  $\{u\}^{ddl}$  and values defined under the keyword THM\_INIT that we call  $p^{ref}$  and  $T^{ref}$

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

Significance of the unknown factors PRE1 and PRE2 vary according to the models. While noting  $p_w$  water pressure,  $p_{ad}$  dissolved air pressure,  $p_{lq}$  pressure of liquid  $p_{lq} = p_w + p_{ad}$ ,  $p_{as}$ ,  $p_{vp}$  the steam pressure,  $p_{as}$  the air pressure dryness and  $p_g = p_{as} + p_{vp}$  total gas pressure and  $p_c = p_g - p_{lq}$  the capillary pressure (also called suction), one has the following meanings of the unknown factors PRE1 and PRE2

Behavior KIT	LIQU_SATU	LIQU_GAZ_ATM	GAS	LIQU_VAPE_GAZ
PRE1	$p_{lq}$	$-p_{lq}$	$p_g$	$p_c = p_g - p_{lq}$
PRE2				$p_g$

Behavior KIT	LIQU_GAZ	LIQU_VAPE	LIQU_AD_GAZ_VAPE or LIQU_AD_GAZ
PRE1	$p_c = p_g - p_{lq}$	$p_{lq}$	$p_c = p_g - p_{lq}$
PRE2	$p_g$		$p_g$

**Table 2.2.3-1: contents of PRE1 and PRE2**

One then defines the "total" pressures and the temperature by:

$$p = p^{ddl} + p^{ref}; T = T^{ddl} + T^{ref}$$

All values as starter or left (boundary conditions or result IMPR\_RESU) are the nodal unknown factors  $p^{ddl}$  et  $T^{ddl}$ .

On the other hand in fact the pressures and the total air temperature are used in the laws of behavior  $\frac{p}{\rho} = \frac{R}{M} T$  for perfect gases,  $\frac{d\rho_l}{\rho_l} = \frac{dp_l}{K_l} - 3\alpha_l dT$  for the liquid and in the relation capillary saturation/pressure.

Let us note that the nodal values can to be initialized by the keyword ETAT\_INIT order STAT\_NON\_LINE (cf 2.3).

The user must be very careful in the definition of the values of THM\_INIT: indeed, the definition of several materials with values different from the quantities defined under THM\_INIT led to discontinuous values initial of the pressure and temperature, which is not in fact not compatible with

the treatment general which is made of these quantities. We thus advise with the user the following approach:

- if there is initially a uniform field of pressure or temperature, one informs it directly by the keyword `THM_INIT`,
- if there is a nonuniform field, one defines for example a reference by the keyword `THM_INIT` order `DEFI_MATERIAU`, and initial values compared to this reference by the keyword `ETAT_INIT` order `STAT_NON_LINE` (cf 2.3).

◇ TEMP

Temperature of reference  $T_{ref}$ . It is necessary for thermal modelings like for all the laws of behavior with gas. For modelings with vapor, it corresponds to the temperature to which is calculated the saturating steam pressure. This value is expressed in Kelvin and must always be strictly positive.

**The value of the temperature of reference entered behind the keyword `TEMP_REF` order `AFFE_MATERIAU` is ignored.**

◆ PRE1

As seen in table 1:

For the behaviors `LIQU_SATU`, and `LIQU_VAPE` pressure of liquid of reference.

For the behavior `GAS` gas pressure of ref.érence. In this case it must be nonworthless.

For the behavior `LIQU_GAZ_ATM` pressure of liquid of changed reference of sign.

For the behaviors `LIQU_VAPE_GAZ`, `LIQU_AD_GAZ`, `LIQU_AD_GAZ_VAPE` and `LIQU_GAZ` capillary pressure of reference.

◇ PRE2

For the behaviors `LIQU_VAPE_GAZ`, `LIQU_AD_GAZ`, `LIQU_AD_GAZ_VAPE` and `LIQU_GAZ` standard gas pressure. This value must be nonworthless.

◆ PORO

Initial porosity.

◆ PRES\_VAPE

Steam pressure of reference for the behaviors: `LIQU_VAPE_GAZ`, `LIQU_AD_GAZ_VAPE` and `LIQU_VAPE`.

**Note:**

*The initial vapor pressure must be taken in coherence with other data. Very often, one leaves the knowledge of an initial state of hygroscoy. 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 pressure of the liquid according to the steam pressure, of the temperature and of saturating steam*

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

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

*$$p_{pv}^{sat}(T_0) = 10^{2.7858 + \frac{T_0 - 273.5}{31.559 + 0.1354(T_0 - 273.5)}}$$*

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

*Moreover, one never should take a value of `PRES_VAPE` equalize to zero.*

## 2.2.3 Keyword factor THM\_LIQU

This keyword relates to all behaviors THM utilizing a liquid (confer [R7.01.11]). Its syntax is the following one:

```
THM_LIQU = _F (
    ♦ RHO                = rho ,          [R]
    ♦ UN_SUR_K           = usk ,          [R]
    ♦ VISC                = VI ,          [function **]
    ♦ D_VISC_TEMP        = dvi ,          [function **]
    ◇ ALPHA              = alp ,          [R]
    ◇ CP                 = CP ,          [R]
)
```

♦ RHO

Density of the liquid for the pressure defined under the keyword PRE1 keyword factor THM\_INIT.

♦ UN\_SUR\_K

Opposite of the compressibility of the liquid:  $K_l$ .

♦ VISC [function \*\*]

Viscosity of the liquid. Function of the temperature.

♦ D\_VISC\_TEMP [function \*\*]

Derived from the viscosity of the liquid compared to the temperature. Function of the temperature. The user must ensure coherence with the function associated with VISC.

◇ ALPHA

Dilation coefficient (linear) of the liquid  $\alpha_l$

If  $p_l$  indicate the pressure of the liquid,  $\rho_l$  its density and  $T$  the temperature, the behavior of

the liquid is: 
$$\frac{d\rho_l}{\rho_l} = \frac{dp_l}{K_l} - 3\alpha_l dT$$

◇ CP

Specific heat with constant pressure of the liquid.

## 2.2.4 Keyword factor THM\_GAZ

This keyword factor relates to all behaviors THM utilizing a gas (cf [R7.01.11]). For the behaviors utilizing at the same time a liquid and a gas, and when one takes into account the evaporation of the liquid, the coefficients indicated here relate to dry gas. The properties of the vapor will be indicated under the keyword THM\_VAPE\_GAZ. Its syntax is the following one:

```
THM_GAZ = _F (
    ♦ MASS_MOL           = Mgs ,          [R]
    ♦ CP                 = CP ,          [R]
    ♦ VISC                = VI ,          [function **]
    ♦ D_VISC_TEMP        = dvi ,          [function **]
)
```

♦ MASS\_MOL

Molar mass of dry gas.  $M_{gs}$

If  $p_{gs}$  indicate the pressure of dry gas,  $\rho_{gs}$  its density,  $R$  the constant of perfect gases and  $T$  the temperature, the reaction of dry gas is: 
$$\frac{p_{gs}}{\rho_{gs}} = \frac{RT}{M_{gs}}$$
.

- ◆ CP  
Specific heat with constant pressure of dry gas.
- ◆ VISC [function \*\*]  
Viscosity of dry gas. Function of the temperature.
- ◆ D\_VISC\_TEMP [function \*\*]  
Derived compared to the temperature from viscosity from dry gas. Function of the temperature.  
The user must ensure coherence with the function associated with VISC.

## 2.2.5 Keyword factor THM\_VAPE\_GAZ

This keyword factor relates to all behaviors THM utilizing at the same time a liquid and a gas, and fascinating of account the evaporation of the liquid (cf [R7.01.11]). The coefficients indicated here relate to the vapor. Syntax is the following one:

```
THM_VAPE_GAZ = _F (
    ◆ MASS_MOL      = m      ,      [R]
    ◆ CP            = CP     ,      [R]
    ◆ VISC          = VI     ,      [function **]
    ◆ D_VISC_TEMP   = dvi    ,      [function **]
)
```

- ◆ MASS\_MOL  
Molar mass of the vapor.  $M_{vp}$
- ◆ CP  
Specific heat with constant pressure of the vapor.
- ◆ VISC [function \*\*]  
Viscosity of the vapor. Function of the temperature.
- ◆ D\_VISC\_TEMP [function \*\*]  
Derived compared to the temperature from viscosity from the vapor. Function of the temperature.  
The user must ensure coherence with the function associated with VISC.

## 2.2.6 Keyword factor THM\_AIR\_DISS

This keyword factor relates to behavior THM THM\_AIR\_DISS taking into account the dissolution of the air in the liquid (cf [R7.01.11]). The coefficients indicated here relate to the dissolved air. Syntax is the following one:

```
THM_AIR_DISS = _F (
    ◆ CP            = CP     ,      [R]
    ◆ COEF_HENRY    = KH     ,      [function **]
)
```

- ◆ CP  
Specific heat with constant pressure of the dissolved air.



◆ COEF\_HENRY

Constant of Henry  $K_H$ , allowing to connect the molar concentration of dissolved air  $C_{ad}^{ol}$  (  $moles/m^3$  ) with the air pressure dryness:

$$C_{ad}^{ol} = \frac{P_{as}}{K_H}$$

**Note:**

The constant of Henry that we use here expresses in  $Pa \cdot m^3 \cdot mol^{-1}$ . In the literature there exist various manners of writing the law of Henry. For example in Benchmarks of Andra, the law of Henry is given by  $\omega_l^a = \frac{P_{as}}{H} \frac{M_{as}^{ol}}{M_w} \rho_w$  with the concentration of air in the water which one can bring back to a density such as  $\omega_l^a = \rho_{ad} \cdot H$ .  $H$  is a coefficient which is expressed in  $Pa$ . It will be necessary in these cases to write equivalence  $K_H = H \frac{M_w}{\rho_w}$

## 2.2.7 Keyword factor THM\_DIFFU

Obligatory for all behaviors THM (cf [R7.01.11]). The user must make sure of the coherence of the functions and their derivative. Syntax is the following one:

Obligatory for all behaviors THM (cf [R7.01.11]). The user must make sure of the coherence of the functions and their derivative.

**Notice important concerning the orthotropism:**

*The user has several possibilities: to place themselves within a classical isotropic framework or to place themselves in a transverse case of isotropy in 3D. In this case it will have to inform a certain number of data materials (cf below) in the directions L and NR of the reference mark of orthotropism, the reference mark L, T being the reference mark of isotropy (cf R4.01.02). In the case 2D, the concept of isotropy transverse loses its direction and in this case only, one places oneself within an orthotropic framework. For the elastic mechanical part one will refer to R4.01.02 and the 3 directions will be to take into account. For the conductive terms (hydraulic and thermal), only the directions L and T of the plan will be this time to be informed (corresponding to reference mark X, Y if the total reference mark coincides with the local reference mark).*

Attention the anisotropy in mechanics is valid only for one elastic mechanical behavior (not programmed for the other laws).

General syntax is the following one:

```
THM_DIFFU = _F (
  ◇ R_GAZ           = rgaz ,           [R]
  ◆ RHO             = rho ,           [R]
  ◇ CP              = CP ,           [R]
  ◆ /BIOT_COEF     = organic ,       [R]
  /|BIOT_L         = biol ,           [R]
  |BIOT_N          = bion ,           [R]
  /|BIOT_T         = biol ,           [R]
  |BIOT_L          = bion ,           [R]
  |BIOT_N          = bion ,           [R]
  ◆ PESA_X         = px ,           [R]
```

```

♦ PESA_Y           = py ,           [R]
♦ PESA_Z           = pz ,           [R]
♦ /PERM_IN         = leave ,         [function]
  /|PERMIN_N       = perml ,         [function]
  |PERMIN_L        = permn ,         [function]
  /|PERMIN_T       = perml ,         [function]
  |PERMIN_L        = permn ,         [function]
♦ /  ◊ SATU_PRES   = sp ,           [function]
  ◊ D_SATU_PRES    = dsp ,           [function]
  ◊ PERM_LIQU      = perml ,         [function]
  ◊ D_PERM_LIQU_SATU = dperm ,       [function]
  ◊ PERM_GAZ       = permg ,         [function]
  ◊ D_PERM_SATU_GAZ = dspg ,         [function]
  ◊ D_PERM_PRES_GAZ = dppg ,         [function]
/  ◊ VG_N          = vgn ,           [R]
  ◊ VG_PR          = Pr ,           [R]
  ◊ VG_SR          = Sr ,           [R]
  ◊ VG_SMAX        = smax ,         [R]
  ◊ VG_SATUR       = stur ,         [R]

◊ FICKV_T         = fvt ,           [function]
◊ FICKV_PV        = / fvpv ,         [function]
  / 1 ,           [DEFECT]
◊ FICKV_PG        = / fvpv ,         [function]
  / 1 ,           [DEFECT]
◊ FICKV_S         = / fvs ,         [function]
  / 1 ,           [DEFECT]
◊ D_FV_T          = / dfvt ,         [function]
  / 0 ,           [DEFECT]
◊ D_FV_PG         = / dfvpg ,        [function]
  / 0 ,           [DEFECT]
◊ FICKA_T         = conceited ,      [function]
◊ FICKA_PA        = / fapv ,         [function]
  / 1 ,           [DEFECT]
◊ FICKA_PL        = / fapg ,         [function]
  / 1 ,           [DEFECT]
◊ FICKA_S         = / fas ,         [function]
  / 1 ,           [DEFECT]
◊ D_FA_T          = / dfat ,         [function]
  / 0 ,           [DEFECT]
◊ /LAMB_T         = / lambt ,        [function]
  / 0 ,           [DEFECT]
  /|LAMB_TN       = / lambt1 ,       [function]
  / 0 ,           [DEFECT]
  |LAMB_TL        = / lambtn ,       [function]
  / 0 ,           [DEFECT]
  /|LAMB_TOUT     = / lambt1 ,       [function]
  / 0 ,           [DEFECT]
  |LAMB_TL        = / lambtn ,       [function]
  / 0 ,           [DEFECT]
◊ LAMB_S          = / lambs ,        [function]
  / 1 ,           [DEFECT]
◊ LAMB_PHI        = / lambp ,        [function]
  / 1 ,           [DEFECT]
◊ /LAMB_CT        = / lambct ,       [function]
  / 0 ,           [DEFECT]
  /|LAMB_C_N      = / lambct1 ,      [function]
  / 0 ,           [DEFECT]
  |LAMB_C_L       = / lambctn ,      [function]

```

```

/ 0 [DEFECT]
/ | LAMB_C_T = / lambctl, [function]
/ 0 [DEFECT]
| LAMB_C_L = / lambctn, [function]
/ 0 [DEFECT]
◇ D_LB_S = / dlambd, [function]
/ 0 [DEFECT]
◇ /D_LB_T = / dlambt, [function]
/ 0 [DEFECT]
/ |D_LB_TN = / dlambtl, [function]
/ 0 [DEFECT]
|D_LB_TL = / dlambtn, [function]
/ 0 [DEFECT]
/ |D_LB_TOUT = / dlambtl, [function]
/ 0 [DEFECT]
|D_LB_TL = / dlambtn, [function]
/ 0 [DEFECT]
◇ D_LB_PHI = / dlambp, [function]
/ 0 [DEFECT]
◇ SIGMA_T = St, [function]
◇ D_SIGMA_T = dst, [function]
◇ PERM_G_INTR = pgi, [function]
◇ CHAL_VAPO = cv, [function **]
◇ EMMAG = EM, [R]
)

```

◆ R\_GAZ

Constant of perfect gases.

◆ RHO

For the hydraulic behaviors initial homogenized density [R7.01.11]. It is that which will intervene in the equilibrium equation of momentum and in the hydraulic part. Attention in the cases with dynamics and only in these cases, it will also be necessary to inform the density in ELAS (the user will have to thus take care of being coherent between these two values).

◇ CP

For the thermal behaviors, specific heat with constant constraint of the solid alone (of the grains).

**Note:**

*Attention it acts here of the specific heat only and not of “  $\rho C_p$  ”, as it is done for other thermal orders. The density of the grains is calculated in the code starting from the homogenized density [R7.01.11].*

◆ BIOT\_COEF

Coefficient of Biot used in the isotropic case.

◆ BIOT\_L, BIOT\_N

In the transverse isotropic case (3D only), the coefficients of Biot for the directions L and NR of the local reference mark of orthotropism. In this case both are obligatory.

◆ BIOT\_L, BIOT\_N, BIOT\_T

In the orthotropic case (in 2D only), the coefficients of Biot for the directions L and NR T. In this case the three are obligatory.

◆ PESA\_X, PESA\_Y, PESA\_Z

Gravity according to X, there and Z

## Note:

*Gravity defined here is that used in the equation of Darcy only. When there are mechanical calculations, gravity is also defined in `AFFE_CHAR_MECA`. This remark applies of course for the three components of gravity.*

◇ `PERM_IN` [function \*\*]

Intrinsic permeability function of porosity in the isotropic case.

The permeability to the classical direction  $K$ , of which dimension is that a speed is calculated in the following way:

$$K = \frac{K_{\text{int}} K_{\text{rel}}}{m} \rho_l g \text{ where } K_{\text{int}} \text{ is the intrinsic permeability, } K_{\text{rel}} \text{ the relative permeability, } m$$

viscosity,  $\rho_l$  density of the liquid and  $g$  the acceleration of gravity. Obligatory in the isotropic case.

◇ `PERMIN_L, PERMIN_N` [function \*\*]

In the isotropic case transverse 3D, the intrinsic permeability for the directions L and NR of the local reference mark of orthotropy. In this case both are obligatory.

◇ `PERMIN_L, PERMIN_T` [function \*\*]

In the orthotropic case in 2D, the intrinsic permeability for the directions L and T of the local reference mark (correspondent with X, Y without rotation of angle). In this case both are obligatory.

◇ `SATU_PRES` [function \*\*]

For the unsaturated material behaviors (`LIQU_VAPE_GAZ, LIQU_VAPE, LIQU_GAZ, LIQU_GAZ_ATM, LIQU_AD_GAZ, LIQU_AD_GAZ_VAPE`), isotherm of saturation function of the capillary pressure. Only for the mixing rates `HYDR_UTIL` or `HYDR_ENDO` (see section 2.5).

## Note:

*For digital reasons, it should be prevented that saturation reaches value 1. Also it is very strongly recommended to multiply the capillary function (generally including between 0 and 1) by 0.999.*

◇ `D_SATU_PRES` [function \*\*]

For the unsaturated material behaviors (`LIQU_VAPE_GAZ, LIQU_VAPE, LIQU_GAZ, LIQU_GAZ_ATM, LIQU_AD_GAZ, LIQU_AD_GAZ_VAPE`), derived from saturation compared to the pressure. Only for the mixing rates `HYDR_UTIL` or `HYDR_ENDO` (see section 2.5).

◇ `PERM_LIQ` [function \*\*]

For the unsaturated material behaviors (`LIQU_VAPE_GAZ, LIQU_VAPE, LIQU_GAZ, LIQU_GAZ_ATM, LIQU_AD_GAZ, LIQU_AD_GAZ_VAPE`), permeability relating to the liquid: function of saturation. Only for the mixing rates `HYDR_UTIL` or `HYDR_ENDO` (see section 2.5).

◇ `D_PERM_LIQ_SATU` [function \*\*]

For the unsaturated material behaviors (`LIQU_VAPE_GAZ, LIQU_VAPE, LIQU_GAZ, LIQU_GAZ_ATM, LIQU_AD_GAZ, LIQU_AD_GAZ_VAPE`), derived from the Permeability relating to the liquid compared to saturation: function of saturation. Only for the mixing rates `HYDR_UTIL` or `HYDR_ENDO` (see section 2.5).

◇ `PERM_GAZ` [function \*\*]

For the unsaturated material behaviors (LIQU\_VAPE\_GAZ, LIQU\_VAPE, LIQU\_GAZ, LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE), permeability relating to gas: function of the saturation and the gas pressure. Only for the mixing rates HYDR\_UTIL or HYDR\_ENDO (see section 2.5).

◇ D\_PERM\_SATU\_GAZ [function \*\*]

For the unsaturated material behaviors (LIQU\_VAPE\_GAZ, LIQU\_VAPE, LIQU\_GAZ, LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE), derived from the permeability to gas by report saturation has: function of the saturation and the gas pressure. Only for the mixing rates HYDR\_UTIL or HYDR\_ENDO (see section 2.5).

◇ D\_PERM\_PRES\_GAZ [function \*\*]

For the unsaturated material behaviors (LIQU\_VAPE\_GAZ, LIQU\_VAPE, LIQU\_GAZ, LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE), derived from the permeability to gas by report has the gas pressure: function of the saturation and the gas pressure. Only for the mixing rates HYDR\_UTIL or HYDR\_ENDO (see section 2.5).

◇ VG\_N [I]

For the unsaturated material behaviors with two unknown factors ( LIQU\_VAPE\_GAZ , LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE , LIQU\_GAZ) and if the hydraulic law is HYDR\_VGM or HYDR\_VGC (see section 2.5 ), indicate the parameter  $N$  law of Mualem Van-Genuchten being used to define the capillary pressure and the permeabilities relating to water and gas.

◇ VG\_PR [R]

For the unsaturated material behaviors with two unknown factors ( LIQU\_VAPE\_GAZ , LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE , LIQU\_GAZ) and if the hydraulic law is HYDR\_VGM or HYDR\_VGC (see section 2.5 ), the parameter indicates  $P_r$  law of Mualem Van-Genuchten being used to define the capillary pressure and the permeabilities relating to water and gas.

◇ VG\_SR [R]

For the unsaturated material behaviors with two unknown factors ( LIQU\_VAPE\_GAZ , LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE , LIQU\_GAZ) and if the hydraulic law is HYDR\_VGM or HYDR\_VGC (see section 2.5 ), the parameter indicates  $S_r$  of residual saturation of the law of Mualem Van-Genuchten being used to define the capillary pressure and the permeabilities relating to water and gas.

◇ VG\_SMAX [R]

For the unsaturated material behaviors with two unknown factors ( LIQU\_VAPE\_GAZ , LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE , LIQU\_GAZ) and if the hydraulic law is HYDR\_VGM or HYDR\_VGC (see section 2.5 ), indicates the maximum saturation for which one applies the law of Mualem Van-Genuchten. Beyond this saturation the curves of Mualem-Van Genuchten are interpolated. This value must be very close to 1.

◇ VG\_SATUR [R]

For the unsaturated material behaviors with two unknown factors ( LIQU\_VAPE\_GAZ , LIQU\_AD\_GAZ, LIQU\_AD\_GAZ\_VAPE , LIQU\_GAZ) and if the hydraulic law is HYDR\_VGM or HYDR\_VGC (see section 2.5 ). Beyond the saturation defined by VG\_SMAX, saturation is multiplied by this corrective factor. This value must be very close to 1 (see Doc. R7.01.11).

◇ FICKV\_T [function \*\*]

For the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE, multiplicative part of the coefficient of Fick function of the temperature for the diffusion of the vapor in the gas mixture. The coefficient of Fick which can be a function of saturation, the temperature, the pressure of gas and the steam pressure, one defines it as a product of 4 functions: FICKV\_T, FICKV\_S, FICKV\_PG,

FICKV\_VP. Only FICKV\_T is obligatory for the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE. See remark in section 2.2.8.

◇ FICKV\_S [function \*\*]

For the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE, multiplicative part of the coefficient of Fick function of saturation for the diffusion of the vapor in the gas mixture. If this function is used, one recommends to take FICKV\_S (1) = 0. See remark in section 2.2.8.

◇ FICKV\_PG [function \*\*]

For the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE, multiplicative part of the coefficient of Fick function of the gas pressure for the diffusion of the vapor in the gas mixture. See remark in section 2.2.8.

◇ FICKV\_PV [function \*\*]

For the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE, multiplicative part of the coefficient of Fick function of the steam pressure for the diffusion of the vapor in the gas mixture. See remark in section 2.2.8.

◇ D\_FV\_T [function \*\*]

For the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE, derived from the coefficient FICKV\_T compared to the temperature. See remark in section 2.2.8.

◇ D\_FV\_PG [function \*\*]

For the behaviors LIQU\_VAPE\_GAZ and LIQU\_AD\_GAZ\_VAPE, derived from the coefficient FICKV\_PG compared to the gas pressure. See remark in section 2.2.8.

◇ FICKA\_T [function \*\*]

For the behavior LIQU\_AD\_GAZ\_VAPE and LIQU\_AD\_GAZ, multiplicative part of the coefficient of Fick function of the temperature for the diffusion of the air dissolved in the liquid mixture. The coefficient of Fick which can be a function of saturation, the temperature, the dissolved air pressure and the pressure of liquid, one defines it as a product of 4 functions: FICKA\_T, FICKA\_S, FICKV\_PA, FICKV\_PL. In the case of LIQU\_AD\_GAZ\_VAPE, only FICKA\_T is obligatory. See remark in section 2.2.8.

◇ FICKA\_S [function \*\*]

For the behavior LIQU\_AD\_GAZ\_VAPE and LIQU\_AD\_GAZ, multiplicative part of the coefficient of Fick function of saturation for the diffusion of the air dissolved in the liquid mixture. See remark in section 2.2.8.

◇ FICKA\_PA [function \*\*]

For the behavior LIQU\_AD\_GAZ\_VAPE and LIQU\_AD\_GAZ, multiplicative part of the coefficient of Fick function of the air pressure dissolved for the diffusion of the air dissolved in the liquid mixture. See remark in section 2.2.8.

◇ FICKA\_PL [function \*\*]

For the behavior LIQU\_AD\_GAZ\_VAPE and LIQU\_AD\_GAZ, multiplicative part of the coefficient of Fick function of the pressure of liquid for the diffusion of the air dissolved in the liquid mixture. See remark in section 2.2.8.

◇ D\_FA\_T [function \*\*]

For the behavior LIQU\_AD\_GAZ\_VAPE and LIQU\_AD\_GAZ, derived from the coefficient FICKA\_T compared to the temperature. See remark in section 2.2.8.

◇ LAMB\_T [function \*\*]

Multiplicative part of the thermal conductivity of the mixture depend on the temperature (See remark in section 2.2.8.). This operand is obligatory in the thermal and isotropic case.

◇ LAMB\_TL, LAMB\_TN [function \*\*]

In the transverse isotropic case, multiplicative parts of the thermal conductivity of the mixture depend on the temperature for the directions L and NR of the local reference mark of orthotropism. These operands are obligatory if there is thermics in transverse isotropy.

◇ LAMB\_TL, LAMB\_TOUT [function \*\*]

In the orthotropic case 2D, left multiplicative the thermal conductivity of the mixture depend on the temperature for the directions L and T. These operands are obligatory if there is thermics in orthotropism.

◇ LAMB\_S [function \*\*]

Multiplicative part (equal to 1 by default) of the thermal conductivity of the mixture depend on saturation (See remark in section 2.2.8).

◇ LAMB\_PHI [function \*\*]

Multiplicative part (to 1 by default equalizes) thermal conductivity of the mixture depend on porosity (cf [§2.2.9]).

◇ LAMB\_CT [function \*\*]

Part of the thermal of the constant mixture and additive conductivity in the isotropic case (cf [§2.2.9]). This constant is equal to zero by default.

◇ LAMB\_C\_L, LAMB\_C\_N [function \*\*]

In the transverse isotropic case, left the thermal conductivity of the constants mixture and additive (cf [§2.2.9]) for the directions L and NR of the local reference mark of orthotropism. These constants are equal to zero by default.

◇ LAMB\_C\_L, LAMB\_C\_T [function \*\*]

In the orthotropic case 2D, left the thermal conductivity of the constants mixture and additive (cf [§2.2.9]) for the directions L and T of the local reference mark. These constants are equal to zero by default.

◇ D\_LB\_T [function \*\*]

Derived from the part of thermal conductivity of the mixture depend on the temperature compared to the temperature in the isotropic case.

◇ D\_LB\_TL, D\_LB\_TN [function \*\*]

In the transverse isotropic case, derived from the parts of thermal conductivity of the mixture depend on the temperature compared to the temperature, for the directions L and NR of the local reference mark of orthotropism.

◇ D\_LB\_TL, D\_LB\_TOUT [function \*\*]

In the orthotropic case 2D, derived from the parts of thermal conductivity of the mixture depend on the temperature compared to the temperature, for the directions L and TN of the local reference mark of orthotropism.

◇ D\_LB\_S [function \*\*]

Derived from the part of thermal conductivity of the mélange depend on saturation.

◇ D\_LB\_PHI [function \*\*]

Derived from the part of thermal conductivity of the mixture depend on porosity.

◇ EMMAG [function \*\*]

Coefficient of storage. This coefficient is taken into account only in the cases of modelings without mechanics.

**Note:**

*Attention it is important to remind the user that the parameters `BIOT_COEF` and `BIOT_L`, `BIOT_N` are incompatible for the same modeling. The user must inform the parameter `BIOT_COEF` if it chooses to conduct a study in the isotropic case, parameters `BIOT_L`, `BIOT_N` if it chooses to conduct its study in isotropic transverse, or `BIOT_L`, `BIOT_N` and `BIOT_T` in the orthotropic case 2D. The same rule is applicable for the parameters `PERM_IN`, `LAMB_T`, `D_LB_T` and `LAMB_CT`. For these conductive terms, in the orthotropic case 2D, only the components `L` and `T` are necessary.*

## 2.2.8 Summary of the functions of couplings and their dependence

The tables below point out the various functions and their possible dependences and obligations.

### Keyword factor `THM_LIQU`

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

### Keyword factor `THM_GAZ`

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

### Keyword factor `THM_VAPE_GAZ`

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

### Keyword factor `THM_AIR_DISS`

◆	CP	$C_{ad}^p$
◆	COEF_HENRY	$K_H$



## Keyword factor THM\_INIT

◇	TEMP	$init T$
◆	PRE1	$init P_1$
◇	PRE2	$init P_2$
◆	PORO	$\Phi^0$
◇	NEAR_VAPE	$p_{vp}^0$

## •Keyword factor THM\_DIFFU

◇	R_GAZ	$R$
◆	RHO	$r_0$
◇	CP	$C_\sigma^s$
◇	BIOT_COEF	$b$
◇	BIOT_L	$b_L$
◇	BIOT_N	$b_N$
◇	BIOT_T	$b_T$
◇	SATU_PRES	$S_{lq}(p_c)$
◇	D_SATU_PRES	$\frac{\partial S_{lq}(p_c)}{\partial p_c}$
◆	PESA_X	$F_x^m$
◆	PESA_Y	$F_y^m$
◆	PESA_Z	$F_z^m$
◇	PERM_IN	$K^{int}(\Phi)$
◇	PERMIN_L	$K^{int}(\Phi)$ according to L
◇	PERMIN_N	$K^{int}(\Phi)$ according to NR
◇	PERMIN_T	$K^{int}(\Phi)$ according to T (2D)
◇	PERM_LIQU	$k_{lq}^{rel}(S_{lq})$
◇	D_PERM_LIQU_SATU	$\frac{\partial k_{lq}^{rel}(S_{lq})}{\partial S_{lq}}$
◇	PERM_GAZ	$k_{gz}^{rel}(S_{lq}, p_{gz})$
◇	D_PERM_SATU_GAZ	$\frac{\partial k_{gz}^{rel}(S_{lq}, p_{gz})}{\partial S_{lq}}$
◇	D_PERM_PRES_GAZ	$\frac{\partial k_{gz}^{rel}(S_{lq}, p_{gz})}{\partial p_{gz}}$
◇	FICKV_T	$f_{vp}^T(T)$
◇	FICKV_S	$f_{vp}^S(S)$

◇	FICKV_PG	$f_{vp}^{gz}(P_g)$
◇	FICKV_PV	$f_{vp}^{vp}(P_{vp})$
◇	D_FV_T	$\frac{\partial f_{vp}^T(I)}{\partial T}$
◇	D_FV_PG	$\frac{\partial f_{vp}^{gz}(P_{gz})}{\partial P_{gz}}$
◇	FICKA_T	$f_{ad}^T(T)$
◇	FICKA_S	$f_{ad}^S(S)$
◇	FICKA_PA	$f_{ad}^{ad}(P_{ad})$
◇	FICKA_PL	$f_{ad}^{lq}(P_{lq})$
◇	D_FA_T	$\frac{\partial f_{ad}^T(I)}{\partial T}$
◇	LAMB_T	$\lambda_T^T(T)$
◇	LAMB_TL	$\lambda_T^T(T)$ according to L
◇	LAMB_TN	$\lambda_T^T(T)$ according to NR
◇	LAMB_TT	$\lambda_T^T(T)$ according to T (2D)
◇	D_LB_T	$\frac{\partial \lambda_T^T(T)}{\partial T}$
◇	D_LB_TL	$\frac{\partial \lambda_T^T(T)}{\partial T}$ according to L
◇	D_LB_TN	$\frac{\partial \lambda_T^T(T)}{\partial T}$ according to NR
◇	D_LB_TT	$\frac{\partial \lambda_T^T(T)}{\partial T}$ according to T (2D)
◇	LAMB_PHI	$\lambda_\phi^T(\phi)$
◇	D_LB_PHI	$\frac{\partial \lambda_\phi^T(\phi)}{\partial \phi}$
◇	LAMB_S	$\lambda_S^T(S)$
◇	D_LB_S	$\frac{\partial \lambda_S^T(S)}{\partial S}$
◇	LAMB_CT	$\lambda_{CT}^T$
◇	LAMB_C_L	$\lambda_{CT}^T$ according to L
◇	LAMB_C_N	$\lambda_{CT}^T$ according to NR
◇	LAMB_C_T	$\lambda_{CT}^T$ according to T (2D)

**Note:**

If there is thermics:

$\lambda^T$  is function of porosity, saturation and temperature and is given in the shape of the product of three functions:

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$\lambda^T = \lambda_\phi^T(\phi) \cdot \lambda_S^T(S_{lq}) \cdot \lambda_T^T(T) + \lambda_{cte}^T$  with the tensor  $\lambda_T^T(T)$  obligatory and the other functions by default taken equal to one, except the tensor  $\lambda_{cte}^T = \mathbf{0}$ .

For the coefficient of Fick of the gas mixture, in the case `LIQU_VAPE_GAZ` and `LIQU_AD_GAZ_VAPE`  $F_{vp}(P_{vp}, P_{gz}, T, S) = f_{vp}^{vp}(P_{vp}) \cdot f_{vp}^{gz}(P_{gz}) \cdot f_{vp}^T(T) \cdot f_{vp}^S(S)$  with  $f_{vp}^T(T)$  obligatory, other functions being taken by default equal to one, and their derivative equal to zero. One will neglect the derivative compared to steam pressure and saturation.

In the cases `LIQU_AD_GAZ_VAPE` and `LIQU_AD_GAZ`, the coefficient of Fick of the liquid mixture will be in the form:  $F_{ad}(P_{ad}, P_{lq}, T, S) = f_{ad}^{ad}(P_{ad}) \cdot f_{ad}^{lq}(P_{lq}) \cdot f_{ad}^T(T) \cdot f_{ad}^S(S)$ , with  $f_{ad}^T(T)$  obligatory, other functions being taken by default equal to one, and their derivative equalizes to zero. One considers only the derivative compared to the temperature (the others are in any case taken equal to zero).

## 2.3 Initialization of calculation

To define an initial state, it is necessary to define a state of generalized stresses (with the elements), nodal unknown factors and internal variables.

- In the keyword `THM_INIT` of `DEFI_MATERIAU`, one defines values of reference for the nodal unknown factors.
- By the keyword `DEPL` keyword factor `ETAT_INIT` order `STAT_NON_LINE`, one affects the field of initialization of the nodal unknown factors.
- By the keyword `SIGM` keyword factor `ETAT_INIT` order `STAT_NON_LINE`, the fields of initialization of the constraints are affected.
- By the keyword `VARI` keyword factor `ETAT_INIT` one affects (possibly) the fields of initialization of the internal variables.

In order to specify the things, one recalls to which category of variables belongs each physical size (these physical sizes existing or not according to selected modeling):

<b>Nodal unknown factors</b>	$p_c, p_g, p_{lq}, T, u_x, u_y, u_z$
<b>Constraints at the points of Gauss</b>	$\sigma'_{xx}, \sigma'_{yy}, \sigma'_{zz}, \sigma'_{xy}, \sigma'_{xz}, \sigma'_{yz}, \sigma'_{p_{xx}}, \sigma'_{p_{yy}}, \sigma'_{p_{zz}}, \sigma'_{p_{xy}}, \sigma'_{p_{xz}}, \sigma'_{p_{yz}},$ $m_w, M_{w_x}, M_{w_y}, M_{w_z}, m_{vp}, M_{vp_x}, M_{vp_y}, M_{vp_z}, m_{as}, M_{as_x}, M_{as_y}, M_{as_z},$ $m_{ad}, M_{ad_x}, M_{ad_y}, M_{ad_z}, h_w^m, h_{vp}^m, h_{as}^m, h_{ad}^m, Q', q_x, q_y, q_z$
<b>Internal variables</b>	$\phi, \rho_{lq}, p_{vp}, S_{lq}$

The correspondence between name of component Aster and physical size is clarified in [§Annexe 1]. The initialization of the nodal unknown factors as well as the difference between initial state and state in reference were described and detailed in the section 2.2.2. It is pointed out nevertheless that  $p = p^{ddl} + p^{ref}$  for the pressures `PRE1` and `PRE2` and  $T = T^{ddl} + T^{ref}$  for the temperatures, where  $p^{ref}$  and  $T^{ref}$  are defined under the keyword `THM_INIT` order `DEFI_MATERIAU`.

The keyword `DEPL` keyword factor `ETAT_INIT` order `STAT_NON_LINE` defines the initial values of  $\{u\}^{ddl}$ . 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  $u = u^{ddl} + u^{ref}$  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`.

Concerning the constraints, the fields to be informed are the constraints indicated in appendix I following selected modeling.

Initial values of the enthalpi, which belong to the generalized constraints are defined starting from the keyword `SIGM` keyword factor `ETAT_INIT` order `STAT_NON_LINE`. The introduction of the initial conditions is very important, for the enthalpi. In practice, one can reason by considering that one has three states for the fluids:

- the state running,
- the state of reference: it is that of the fluids in a free state. In this state of reference, one can consider that the enthalpi are worthless,
- the initial state: it must be in thermodynamic balance. For the enthalpi of water and vapor, one will have to take:

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

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

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

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

and with  $L(T) = 2500800 - 2443(T - 273.15)$  J/kg

**Note:**

The initial vapor pressure will have to be taken in coherence with these choices (cf 2.2.3).

Concerning the mechanical constraints, the partition of the constraints in constraints total and effective is written:

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

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

$\sigma'$  is the effective constraint. For the laws of effective constraints:  $d\sigma' = f(d\varepsilon - \alpha_0 dT, \alpha)$ ,

where  $\varepsilon = \frac{1}{2}(\nabla u + {}^T\nabla u)$  and  $\alpha$  represent the internal variables.

Components of the tensor  $\sigma_p$  are calculated according to the water pressures. The adopted writing is incremental and, if it is wanted that the value of the components of  $\sigma_p$  are coherent with the value  $p^{ref}$  (PRE1) defined under the keyword THM\_INIT, it is necessary to initialize the components of  $\sigma_p$  by the keyword SIGM keyword factor ETAT\_INIT order STAT\_NON\_LINE.

Example:

Fields of displacements initialized in ETAT\_INIT can be in the following way defined:

```
CHAMNO=CRÉA_CHAMP (MAILLAGE=MAIL,
                    OPERATION=' AFFE ',
                    TYPE_CHAM=' NOEU_DEPL_R ',
                    AFFE= ( _F (TOUT=' OUI ',
                                NOM_CMP=' TEMP ',
                                VALE=0.0, ),
                            _F (GROUP_NO=' SURFBO ',
                                NOM_CMP=' PRE1 ',
                                VALE=7.E7, ),
                            _F (GROUP_NO=' SURFBG ',
                                NOM_CMP=' PRE1 ',
                                VALE=3.E7, ),
                            _F (GROUP_NO=' SURFBO ',
                                NOM_CMP=' PRE2 ',
                                VALE=0.0, ),
                            _F (GROUP_NO=' SURFBG ',
                                NOM_CMP=' PRE2 ',
                                VALE=0.0, ), ), );
```

And stress fields in the following way:

```
SIGINIT=CRÉA_CHAMP (MAILLAGE=MAIL,
                    OPERATION=' AFFE ',
                    TYPE_CHAM=' CART_SIEF_R ',
```

```

AFFE= (_F (GROUP_MA=' BO',
          NOM_CMP=
('SIXX', 'SIYY', 'SIZZ', 'SIXY', 'SIXZ',
 'SIYZ', 'SIPXX', 'SIPYY', 'SIPZZ', 'SIPXY',
 'SIPXZ', 'SIPYZ',
 'M11', 'FH11X', 'FH11Y', 'ENT11',
 'M12', 'FH12X', 'FH12Y', 'ENT12',
 'QPRIM', 'FHTX', 'FHTY', 'M21',
 'FH21X', 'FH21Y', 'ENT21',
 'M22', 'FH22X', 'FH22Y', 'ENT22',)),
VALE=
(0.0, 0.0, 0.0, 0.0, 0.0,
 0.0,0.0, 0.0, 0.0, 0.0,
 0.0,0.0,
 0.0,0.0, 0.0, 0.0,
 0.0,0.0, 0.0, 2500000.0,
 0.0,0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
 0. , 0. , 0. , 0.),),),);

```

## 2.4 Loadings and boundary conditions

All the boundary conditions or loading are affected via the order `AFFE_CHAR_MECA` [U4.44.01]. The loadings are then activated by the keyword factor `EXCIT` order `STAT_NON_LINE`.

In a classical way, two types of boundary conditions are possible:

- Conditions of the Dirichlet type which consist in imposing on part of border of the values fixed for principal unknown factors belonging to  $\{u\}^{ddl}$  (and not  $u = u^{ddl} + u^{init}$ ) for that one uses the keyword factor `DDL_IMPO` or `FACE_IMPO` of `AFFE_CHAR_MECA`.
- Conditions of the Neumann type which consist in imposing values on the “dual quantities”, either by not saying anything (worthless flows in hydraulics and thermics), or in their giving a value via the keywords `FLUN`, `FLUN_HYDR1` and `FLUN_HYDR2` keyword factor `FLUX_THM_REP` order `AFFE_CHAR_MECA`. This flow is then multiplied by a function of time (by default equalizes to 1) called by `FONC_MULT` under keyword `EXCIT` order `STAT_NON_LINE`. `FLUN`, `FLUN_HYDR1` and `FLUN_HYDR2` the heat fluxes, water flows and flows of gas component represent respectively (cf, end of the paragraph).
- Mechanical conditions in total constraints  $\sigma.n$  are they given via `PRES_REP` order `AFFE_CHAR_MECA`. One will refer to the documentation of this order to know the possibilities of them.

From a syntactic point of view the conditions of Dirichlet thus apply as to the following example

```

DIRI=AFFE_CHAR_MECA (MODELE=MODELE,
                    DDL_IMPO= (_F (GROUP_NO=' GAUCHE',
                                  TEMP=0.0,)),
                        _F (TOUT=' OUI',
                            PRE2=0.0,)),
                    _F (GROUP_NO=' GAUCHE',
                        PRE1=0.0,)),
                    _F (TOUT=' OUI',
                        DX=0.0,)),
                    _F (TOUT=' OUI',
                        DY=0.0,)),
                    _F (TOUT=' OUI',
                        DZ=0.0,)),
                    ),)

```

For the conditions of Neuman, syntax will be then as on the following example:

```
NEU1=AFFE_CHAR_MECA (MODELE=MODELE,
                    FLUX_THM_REP=_F (GROUP_MA=' DROIT',
                    FLUN=200.,
                    FLUN_HYDR1=0.0,
                    FLUN_HYDR2=0.0),);
NEU2=AFFE_CHAR_MECA (MODELE=MODELE,
                    PRES_REP=_F (GROUP_MA=' DROIT',
                    PRES=2.,),);
```

One defines then the multiplicative function which one wants to apply, for example with *NEU1* :

```
FLUX=DEFI_FONCTION (NOM_PARA=' INST',
                   VALE=
                   (0.0, 386.0,
                   315360000.0, 312.0,
                   946080000.0, 12.6),);
```

The loadings are then activated in *STAT\_NON\_LINE* via the keyword *EXCIT* in the following way:

```
EXCIT= (
        _F (CHARGE=DIRI, ),
        _F (CHARGE=NEU2, ),
        _F (CHARGE=NEU1,
            FONC_MULT=FLUX, ),
        ),
```

*FLUN* corresponds to the value of the heat flow; *FLUN\_HYDR1* and *FLUN\_HYDR2* correspond to the values of the hydraulic flows associated with the pressures *PRE1* and *PRE2*. If there is no ambiguity for thermics or mechanics, on the other hand hydraulic principal unknown factors *PRE1* and *PRE2* change according to the selected coupling. As it below is pointed out

Behavior	LIQU_SATU	LIQU_VAPE	LIQU_GAZ_ATM	GAS	LIQU_VAPE_GAZ LIQU_GAZ LIQU_AD_GAZ_VA PE LIQU_AD_GAZ
<i>PRE1</i>	$P_{lq}$	$P_{lq}$	$-P_{lq}$	$P_g$	$P_c = P_g - P_{lq}$
<i>PRE2</i>					$P_g$

Associated flows are:

$$\text{For } PRE1, FLUN\_HYDR1 : (M_w + M_{vp}) \cdot n = M_w^{ext} + M_{vp}^{ext}$$

$$\text{For } PRE2, FLUN\_HYDR2 : (M_{ad} + M_{as}) \cdot n = M_{ad}^{ext} + M_{as}^{ext}$$

We will thus summarize the various possibilities by distinguishing the case where one imposes values on *PRE1* and/or *PRE2* and that where one works on combinations of the 2. It is announced that one can of course have various types of boundary conditions according to the pieces of border (groups of nodes or meshes) which one treats. For a more complete and more detailed outline in the way in which are treated the boundary conditions in the case unsaturated, one will refer to the note reproduced in appendix 2.

- **Case of the boundary conditions utilizing principal unknown factors *PRE1* and *PRE2***

One summarizes the usual case here where one imposes values on *PRE1* and/or *PRE2*.

- Dirichlet on `PRE1` and Dirichlet on `PRE2`  
The user imposes a value on `PRE1` and `PRE2` ; flows are computation results.
  - Dirichlet on `PRE1` and Neuman on `PRE2`  
The user imposes a value on `PRE1` and a value with flow associated with `PRE2` by not saying anything on `PRE2` or by giving a value to `FLUN_HYDR2`.
  - Dirichlet on `PRE2` and Neuman on `PRE1`  
The user imposes a value on `PRE2` and a value with flow associated with `PRE1` by not saying anything on `PRE1` or by giving a value to `FLUN_HYDR1`.
  - Neuman on `PRE2` and Neuman on `PRE1`  
Two flows are imposed either by not saying anything on `PRE1` and/or `PRE2` (worthless flows) that is to say by giving a value to `FLUN_HYDR1` and/or `FLUN_HYDR2`
- **Case of the boundary conditions utilizing a linear relation between the principal unknown factors `PRE1` and `PRE2`**

It is also possible to handle linear combinations of `PRE1` and `PRE2`. It is necessary however to handle that with precaution so as to start from a correctly posed problem. The syntax of this operator is detailed in the documentation of `AFPE_CHAR_MECA`, the example below illustrates this kind of condition:

```
P_DDL=AFPE_CHAR_MECA (MODELE=MODELE,  
                      LIAISON_GROUP= (_F (  
                                      GROUP_NO_1= 'EDGES',  
                                      GROUP_NO_2= 'EDGES',  
                                      DDL_1=' PRE1',  
                                      DDL_2=' PRE2',  
                                      COEF_MULT_1 = X,  
                                      COEF_MULT_2 = Y.,  
                                      COEF_IMPO =z,)),),  
                      );
```

This order means that on the border defined by the group of nodes `BORDS`, pressures `PRE1` and `PRE2` are connected by the linear relation

$$x PRE1 + y PRE2 = z$$

**Note:**

Imposed flows are scalar quantities which can apply to a line or an internal surface to the modelled solid. In this case, these boundary conditions correspond to a source.

## 2.5 Nonlinear calculation

The resolution can be carried out in 2 manners:

- 1.method of the coupling: it is most reliable, most robust and oldest
- 2.method of the chaining: it is a new strategy, adapted for the slightly coupled problems and the problems not being able to be currently solved by the method of the coupling.

Ex:

- calculation with the mechanical law of behavior 'ENDO\_HETEROGENE', which is not available in kit THM
- calculation with diphasic hydraulic modelings in finished volumes, which are not available in kit THM coupled with mechanics

The heart of the resolution is the order 'STAT\_NON\_LINE'. To this order one assigns the model (keyword `MODEL`), the materials (keyword `CHAM_MATER`), le/les loadings (keyword `EXCIT`) and the initial state (keyword `ETAT_INIT`) that one defined by all the orders described previously.



For general information concerning this order and his syntax, one will refer to his documentation. It is specified just that the method of calculating is a method of Newton. One does not speak thus below that of what is specific to calculations THM with knowing the keywords factors `RELATION` and `RELATION_KIT` keyword `BEHAVIOR` who are closely dependent.

**Caution:**

Under the keyword factor `NEWTON`, one must put a matrix of the type '`TANGENT`' and not '`ELASTIC`' .

One presents initially examples of use for the two strategies of resolution.

## 2.5.1 Resolution by coupling

In this case, the resolution is carried out by only one orders `STAT_NON_LINE` :

```
U0=STAT_NON_LINE (MODELE=MODELE,  
                  CHAM_MATER=CHMAT0,  
                  EXCIT= (  
                      _F (CHARGE=T_IMP, ),  
                      _F (CHARGE=CALINT,  
                          FONC_MULT=FLUX, ), ),  
                  COMPORTEMENT=_F (RELATION=' KIT_THHM',  
                                    RELATION_KIT=  
                                    ('ELAS', 'LIQU_GAZ', 'HYDR_UTIL'), ),  
                  ETAT_INIT=_F (DEPL=CHAMNO,  
                                 SIGM=SIGINIT),  
                  INCREMENT=_F (LIST_INST=INST1, ),  
                  NEWTON=_F (MATRICE=' TANGENTE', REAC_ITER=1, ),  
                  CONVERGENCE=_F (RESI_GLOB_RELA=1.E-06,  
                                   ITER_GLOB_MAXI=15,  
                                   ITER_INTE_MAXI=5, ),  
                  ARCHIVAGE=_F (PAS_ARCH=1, ), );
```

## 2.5.2 Resolution by chaining

The resolution by chaining currently applies to the only saturated Hydro-mechanical problems. One points out initially the equations of this problem:

$$\begin{aligned} -\nabla \cdot \sigma'(u) + b \nabla p &= 0 \\ \partial_t(\rho \phi) + \nabla \cdot M_{lq} &= 0 \end{aligned}$$

where porosity  $\phi$  the law of behavior follows  $d\phi = bd(\nabla \cdot u) + \frac{b-\phi}{K_s} dp$ .

Within the framework of the chaining, one solves separately the problems mechanics and hydraulics. The communication between two calculations is carried out via variables of order ('`PTOT`' and '`DIVU`'). For the mechanical problem, the variable of order '`PTOT`' play the part of the data of pressure. For the hydraulic problem, the variable of order '`DIVU`' play the part of the voluminal data of deformation.

These variables of order are calculated by the order `CHAINAGE_THM`.

The method illustrated below is a basic algorithm of pure chaining of calculations (hydraulic resolution at moment 1, mechanical resolution at moment 1, hydraulic resolution at moment 2, mechanical resolution at moment 2, etc...). One could consider more complicated algorithms (of type not fixes or nonlinear combined gradient) but that complexes of as much the setting in data in the command file. The question of the convergence of such algorithms is not either whole not acquired!

The final mechanical solution is `DEPLA` and hydraulic solution is `PRELIQ`.

```
# buckles on the steps of time
for K in arranges (1, lenlist):

    UNPAS=DEFI_LISTE_REEL (DEBUT=listinst [k-1],
                          INTERVALLE=_F (JUSQU_A=listinst [K],
                                          NOMBRE=1,));

    UNPASSUB =DEFI_LISTE_INST (DEFI_LIST=_F (LIST_INST =UNPAS),
                                ECHEC=_F (
                                    SUBD_METHODE=' MANUEL',
                                    SUBD_PAS = 4,
                                    SUBD_NIVEAU=5,));

    yew (k>1):

        DEFVHY=CHAINAGE_THM (RESULTAT=DEPLA, INFO=1,
                             MODELE=MODHYD,
                             MATR_PROJECTION=MATPROJ,
                             TYPE_CHAINAGE=' MECA_HYDR',
                             INST=listinst [K,]);

        MATEHY=AFPE_MATERIAU (MAILLAGE=MAIL,
                              AFPE=_F (TOUT=' OUI',
                                       MATER=MATERIAU,)),
                              AFPE_VARC=_F (NOM_VARC=' DIVU',
                                             EVOL=DEFVHY,));

    else:

        MATEHY=AFPE_MATERIAU (MAILLAGE=MAIL,
                              AFPE=_F (TOUT=' OUI',
                                       MATER=MATERIAU,));

    yew (k==1):

        PRELIQ=STAT_NON_LINE (MODELE=MODHYD,
                              CHAM_MATER=MATEHY,
                              EXCIT=_F (CHARGE=CHARHYD,)),
                              SOLVEUR=_F (METHODE=' MUMPS', PCENT_PIVOT=100,)),
                              CONVERGENCE=_F (ITER_GLOB_MAXI=50,)),
                              ARCHIVAGE=_F (LIST_INST=UNPAS,)),
                              COMPORTEMENT=_F (RELATION=' KIT_H',
                                               RELATION_KIT= ('LIQU_SATU',
                                                             'HYDR_UTIL',)),
                              INCREMENT=_F (LIST_INST=UNPASSUB,));

    else:

        PRELIQ=STAT_NON_LINE (reuse=PRELIQ,
                              MODELE=MODHYD,
                              CHAM_MATER=MATEHY,
                              EXCIT=_F (CHARGE=CHARHYD,)),
                              SOLVEUR=_F (METHODE=' MUMPS', PCENT_PIVOT=100,)),
                              ARCHIVAGE=_F (LIST_INST=UNPAS,)),
                              ETAT_INIT=_F (EVOL_NOLI=PRELIQ,
                                             INST=listinst [k-1]),
```

```
CONVERGENCE=_F (ITER_GLOB_MAXI=50,,),
COMPOTEMENT=_F (RELATION=' KIT_H',
                RELATION_KIT= ('LIQU_SATU',
                                'HYDR_UTIL',),),
INCREMENT=_F (LIST_INST=UNPASSUB,,);

yew (k>1):
  TO DESTROY (INFO=1, CONCEPT=_F (NOM= (REPTOT, MATEME,,),),);

REPTOT=CHAINAGE_THM (RESULTAT=PRELIQ,
                    MODELE=MODMEC,
                    TYPE_CHAINAGE=' HYDR_MECA',
                    TYPE_RESU=' EVOL_VARC',
                    INST=listinst [K],);

MATEME=AFFE_MATERIAU (MAILLAGE=MAIL,
                    AFPE=_F (TOUT=' OUI',
                              MATER=MATERIAU,,),
                    AFPE_VARC=_F (TOUT=' OUI',
                                   EVOL=REPTOT,
                                   NOM_VARC=' PTOT',),);

yew (k==1):

  DEPLA=STAT_NON_LINE (MODELE=MODMEC,
                      CHAM_MATER=MATEME,
                      EXCIT=_F (CHARGE=CHARMEC,,),
                      COMPOTEMENT=_F (RELATION=' ELAS',),
                      INCREMENT=_F (LIST_INST=UNPASSUB,,),
                      ARCHIVAGE=_F (LIST_INST=UNPAS,,),
                      NEWTON=_F (MATRICE=' TANGENTE',
                                 REAC_ITER=10,,),
                      CONVERGENCE=_F (ITER_GLOB_MAXI=10,,),
                      SOLVEUR=_F (METHODE=' MUMPS',
                                   PCENT_PIVOT=100,,),);

else:

  DEPLA=STAT_NON_LINE (reuse=DEPLA,
                      MODELE=MODMEC,
                      CHAM_MATER=MATEME,
                      EXCIT=_F (CHARGE=CHARMEC,,),
                      ARCHIVAGE=_F (LIST_INST=UNPAS,,),
                      COMPOTEMENT=_F (RELATION=' ELAS',),
                      ETAT_INIT=_F (EVOL_NOLI=DEPLA,
                                    INST=listinst [k-1]),
                      INCREMENT=_F (LIST_INST=UNPASSUB,,),
                      NEWTON=_F (MATRICE=' TANGENTE',
                                 REAC_ITER=10,,),
                      CONVERGENCE=_F (ITER_GLOB_MAXI=10,,),
                      SOLVEUR=_F (METHODE=' MUMPS',
                                   PCENT_PIVOT=100,,),);

yew (k>1):
  TO DESTROY (INFO=1, CONCEPT=_F (NOM= (DEFVHY,,),),);
  TO DESTROY (INFO=1, CONCEPT=_F (NOM= (UNPAS, UNPASSUB, MATEHY,,),),);
```

## 2.5.3 General advices of use

RELATION is informed by relations of the types `KIT_XXXX` who allow to solve simultaneously from two to four equilibrium equations. The equations considered depend on the suffix `XXXX` with the following rule:

- M indicate the mechanical equilibrium equation,
- T indicate the thermal equilibrium equation,
- H indicate a hydraulic equilibrium equation,
- V indicate the presence of a phase in form vapor (besides the liquid) .

Only one letter *H* mean that the porous environment is saturated (only one variable with pressure  $p$  ), for example either of gas, or of liquid, or of a liquid mixture/gas (of which the pressure of gas is constant).

Two letters *HH* mean that the porous environment is not saturated (two variables with pressure  $p$  ), for example a liquid mixture/vapor/gas.

The presence of the two letters *HV* mean that the porous environment is saturated by a component (in practice of water), but that this component can be in liquid form or vapor. There is not whereas an equation of conservation of this component, therefore only one degree of freedom pressure, but there are a liquid flow and a flow vapor. The possible relations are then the following ones:

```

/   `KIT_HM'
/   `KIT_THM'
/   `KIT_HHM'
/   `KIT_THH'
/   `KIT_THV'
/   `KIT_THHM'
/   `KIT_HH'

```

The table below summarizes to which kit each modeling corresponds:

KIT_HM	D_PLAN_HM, D_PLAN_HMD, D_PLAN_HMS, D_PLAN_HM_SI, AXIS_HM, AXIS_HMD, AXIS_HMS, 3D_HM, 3D_HMD, 3D_HMS, 3D_HM_SI
KIT_THM	D_PLAN_THM, D_PLAN_THMD, D_PLAN_THMS, AXIS_THM, AXIS_THMD, AXIS_THMS, 3D_THM, 3D_THMD, 3D_THMS
KIT_HHM	D_PLAN_HHM, D_PLAN_HHMD, D_PLAN_HHMS, AXIS_HHM, AXIS_HHMD, AXIS_HHMS, 3D_HHM, 3D_HHMD, 3D_HHMS, D_PLAN_HH2MD, AXIS_HH2MD, 3D_HH2MD, D_PLAN_HH2MS, AXIS_HH2MS, 3D_HH2MS, D_PLAN_HH2M_SI, 3D_HH2M_SI
KIT_THH	D_PLAN_THHD, D_PLAN_THHS, AXIS_THHD, AXIS_THHS, 3D_THHD, 3D_THHS, D_PLAN_THH2D, AXIS_THH2D, 3D_THH2D, D_PLAN_THH2S, AXIS_THH2S, 3D_THH2S
KIT_THV	D_PLAN_THVD, AXIS_THVD, 3D_THVD
KIT_THHM	D_PLAN_THHMD, D_PLAN_THHMS, AXIS_THHMD, AXIS_THHMS, 3D_THHM, 3D_THHMD, 3D_THHMS, D_PLAN_THH2MD, AXIS_THH2MD, 3D_THH2MD, D_PLAN_THH2MS, AXIS_THH2MS, 3D_THH2MS
KIT_HH	D_PLAN_HHD, AXIS_HHD, 3D_HHD, D_PLAN_HH2D, AXIS_HH2D, 3D_HH2D, D_PLAN_HHS, AXIS_HHS, 3D_HHS, D_PLAN_HH2S, AXIS_HH2S, 3D_HH2S

For each modelled phenomenon (hydraulic and/or mechanical), one must specify in `RELATION_KIT` :

- The mechanical model of behavior of the skeleton if there is mechanical modeling (M),

```

/   `ELAS'
/   `MOHR_COULOMB'

```

```

/ 'CJS'
/ 'HUJEUX'
/ 'CAM_CLAY'
/ 'BARCELONA'
/ 'LAIGLE'
/ 'LETK'
/ 'DRUCK_PRAGER'
/ 'DRUCK_PRAG_N_A'
/ 'VISC_DRUCK_PRAG'
/ 'ELAS_GONF'
/ 'HOEK_BROWN_TOT'
/ 'HOEK_BROWN_EFF'
/ 'MAZARS'
/ 'ENDO_ISOT_BETON'

```

- The gas/liquid reaction of, (the same one as that indicated in COMP\_THM under DEFINI\_MATERIAU, cf [§2.2.2])

```

/ 'LIQU_SATU'
/ 'LIQU_GAZ'
/ 'GAS'
/ 'LIQU_GAZ_ATM'
/ 'LIQU_VAPE_GAZ'
/ 'LIQU_AD_GAZ_VAPE'
/ 'LIQU_AD_GAZ'
/ 'LIQU_VAPE'

```

- Concerning the hydraulic behavior, the user currently has 4 choices:

```

/ 'HYDR_UTIL'
/ 'HYDR_ENDO'
/ 'HYDR_VGM'
/ 'HYDR_VGC'

```

- Either it chooses HYDR\_UTIL : this keyword then makes it possible to inform the curve of saturation and its derivative according to the capillary pressure as well as the relative permeability and its derivative according to saturation. The user returns these curves via a series of formulas then called by DEFINI\_MATERIAU (cf 2.2.7).
- Either it chooses HYDR\_ENDO : it is the same thing but allows the use of the laws with damage 'MAZARS' and 'ENDO\_ISOT\_BETON' (the permeability is then coupled with the damage).
- Either it chooses HYDR\_VGM or HYDR\_VGC what means that the laws of capillarity and permeabilities will obey the model of preset Mualem-Van-Genuchten in the code, in other words, the capillarity is given by a law of Van Genuchten:

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

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

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 by a law of Parker for HYDR\_VGM :

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

or by a cubic law for HYDR\_VGC :

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

with in all the cases parameters  $n$ ,  $Pr$ ,  $Swr$ ,  $Smax$  defined in DEFI\_MATERIAU :

$n$  corresponds to the parameter VG\_N

$Pr$  corresponds to the parameter VG\_PR

$Swr$  corresponds to the parameter VG\_SR

With that must be added two additional parameters corresponding to a treatment which one carries out on these curves:

$Smax$  who corresponds to the parameter VG\_SMAX

$CSAT$  who corresponds to the parameter VG\_SATUR

We now will clarify what is this treatment and what are  $CSAT$  and  $Smax$ . For  $S > Smax$ , these curves are interpolated by a polynomial of degree 2,  $CI$  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 in the case of HYDR\_VGM:

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

To avoid having 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  $CI$  in this point.

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

For  $S = Smax$ , the polynomial is determined  $PL(S)$  such as

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

For  $S > Smax$ ,  $k_r^w(S)$  is replaced by  $PL(S)$ .

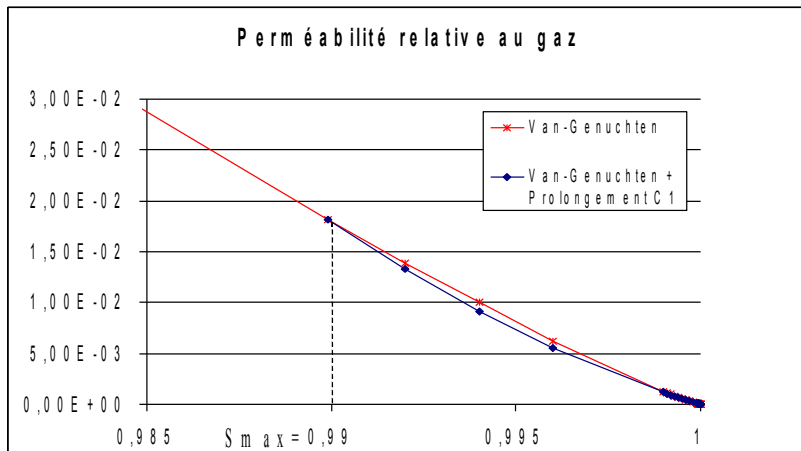
And, in the case of HYDR\_VGM, for  $k_r^{gz}(S)$  :

For  $S = Smax$ , the polynomial is determined  $PG(S)$  such as

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

For  $S > Smax$ ,  $k_r^{gz}(S)$  is replaced by  $PG(S)$  like the example Figure 2.5.3-a. In the case of a cubic law, no special treatment is necessary.





**Figure 2.5.3-a: Example of prolongation of a relative permeability**

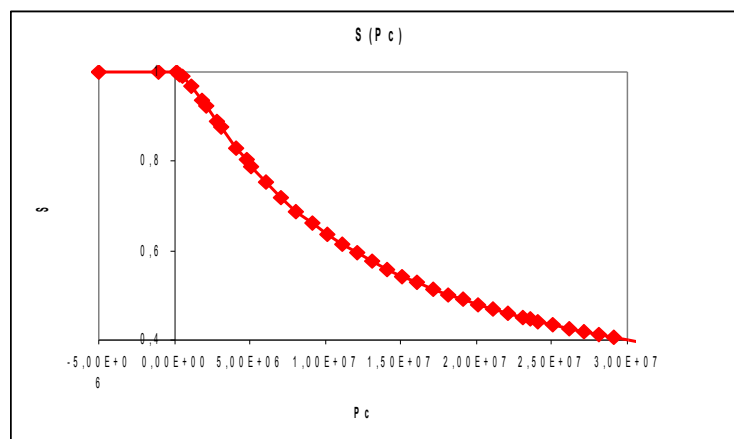
For suction  $S(P_c)$  and for  $P_c < P_{cmin}$  (with  $S(P_{cmin}) = S_{max}$ ) the curve is prolonged  $S(P_c)$  by a hyperbole such as the curve is  $C1$  in this point:

For  $S > S_{max}$  :

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

With  $A$  and  $B$  such that the curve is  $C1$  in  $S_{max}$ .

There is thus well a decreasing curve which tends towards 1 when  $P_c$  tends towards  $-\infty$ . This treatment enables us to manage negative capillary pressures in Code\_Aster (see the example Figure 2.5.3-b).



**Figure 2.5.3-b: Example of prolongation for PC<0**

$S(P_c)$  is then multiplied by a coefficient "of security"  $CSAT$  so that the saturation never reaches 1 (problem which one cannot treat).

**The Council: one advises a value of  $CSAT$  nearest possible to 1 (0,99999 for example).**

**Caution:**



According to *KIT\_XXXX* chosen, all the behaviors are not licit (for example if one selected porous environments unsaturated, one cannot affect one perfect gas reaction of standard). all the possible combinations are summarized below

	Mechanics	Hydraulic coupling	Hydraulic law
KIT_HM KIT_THM	'ELAS', 'MOHR_COULOMB', 'CJS', 'HUJEUX', 'LAIGLE', 'CAM_CLAY', 'DRUCK_PRAGER', 'LEK', 'DRUCK_PRAG_N_A', 'VISC_DRUCK_PRAG', 'ELAS_GONF', 'HOEK_BROWN_TOT', 'HOEK_BROWN_EFF',	'GAS', 'LIQU_SATU', 'LIQU_GAZ_ATM'	'HYDR_UTIL'
KIT_HM KIT_THM	'MAZARS', 'ENDO_ISOT_BETON',	'GAS', 'LIQU_SATU', 'LIQU_GAZ_ATM'	'HYDR_ENDO'
KIT_HHM KIT_THHM	'ELAS', 'MOHR_COULOMB', 'CJS', 'HUJEUX', 'LAIGLE', 'CAM_CLAY', 'DRUCK_PRAGER', 'DRUCK_PRAG_N_A', 'VISC_DRUCK_PRAG', 'ELAS_GONF', 'LEK', 'HOEK_BROWN_TOT', 'HOEK_BROWN_EFF', 'BARCELONA'	'LIQU_GAZ', 'LIQU_VAPE_GAZ', 'LIQU_AD_VAPE_GAZ', 'LIQU_AD_GAZ'	'HYDR_UTIL', 'HYDR_VGM', 'HYDR_VGC'
KIT_HHM KIT_THHM	'MAZARS', 'ENDO_ISOT_BETON',	'LIQU_GAZ', 'LIQU_VAPE_GAZ', 'LIQU_AD_VAPE_GAZ', 'LIQU_AD_GAZ'	'HYDR_ENDO'
KIT_THH KIT_HH		'LIQU_GAZ', 'LIQU_VAPE_GAZ', 'LIQU_AD_VAPE_GAZ', 'LIQU_AD_GAZ'	'HYDR_UTIL', 'HYDR_VGM', 'HYDR_VGC'
KIT_THV		'LIQU_VAPE'	'HYDR_UTIL'

**Note:**

In the event of problem of convergence, it can be very useful to activate linear research. Linear research does not improve however systematically convergence, it is thus to handle with precaution.

## 2.6 Postprocessing

### 2.6.1 General information

The postprocessing of the data in THM does not vary postprocessing usual Aster. It is pointed out just that for any impression of the values to the nodes which are not the nodal unknown factors, it is necessary to calculate these values by the order `CALC_CHAMP` whose one gives an example hereafter.

For the constraints:

```
U0=CALC_CHAMP (reuse =U0,  
               MODELE=MODELE,  
               CHAM_MATER=CHMAT0,  
               TOUT_ORDRE=' OUI',  
               CONSTRAINT= ('SIGM_ELNO'),  
               RESULTAT=U0,);
```

For the internal variables:

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

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```
U0=CALC_CHAMP (reuse =U0,  
               MODELE=MODELE,  
               CHAM_MATER=CHMAT0,  
               TOUT_ORDRE=' OUI ',  
               VARI_INTERNE= ('VARI_ELNO'),  
               RESULTAT=U0,);
```

It should however be recalled that all the values of displacements at exits correspond to  $u^{ddl}$  and not  $u = u^{ddl} + u^{ref}$ .

It is also important to know the name of the constraints and the numbers of the internal variables. All that is consigned in appendix I.

Thus the following example makes it possible to print the liquid water mass on the group of nodes *HAUT* at every moment.

```
TAB1=POST_RELEVE_T (ACTION=_F (INTITULE=' CONT',  
                               GROUP_NO= ('HIGH'),  
                               RESULTAT=U0,  
                               NOM_CHAM=' SIEF_ELNO',  
                               TOUT_ORDRE=' OUI ',  
                               NOM_CMP= ('M11'),  
                               OPERATION=' EXTRACTION',),),);  
  
IMPR_TABLE (TABLE=TAB1,  
            FICHER=' RESULTAT',  
            FORMAT=' AGRAF',  
            PAGINATION=' INST',  
            NOM_PARA= ('INST', 'COOR_X', 'M11'),);
```

The following example makes it possible to print the values of porosity to node 1 and the first moment.

```
TAB2=POST_RELEVE_T (ACTION=_F (INTITULE=' DEPL',  
                               NOEUD=' NO1',  
                               RESULTAT=U0,  
                               NOM_CHAM=' VARI_ELNO',  
                               NUME_ORDRE=1,  
                               NOM_CMP= ('V2'),  
                               OPERATION=' EXTRACTION',),),);  
  
IMPR_TABLE (TABLE=TAB2,  
            FICHER=' RESULTAT',  
            FORMAT=' AGRAF',  
            PAGINATION=' INST',  
            NOM_PARA= ('INST', 'COOR_X', 'V2'),);
```

## 2.6.2 Internal variables

In addition to the general information suggested above, there exists from now on a means more convivial D " of extracting the internal variables (cf Doc. U4.81.01). For that of the fields were created from which the principle is to extract from the field *VARI\_ELGA* (or *VARI\_ELNO* for fields calculated with the nodes) the internal variable which interests us via a keyword more speaking that *V1*, *V2*, ...

As a postprocessing these fields are calculated by *CALC\_CHAMP*. Syntax to be used is the following one:

- for a field with the elements *cham\_elem*

```
GAMP=CALC_CHAMP (RESULTAT=U0,  
  OPTION=' VAEX_ELNO',  
  NOM_VARI=' GAMP');
```

- for a field with the nodes `cham_no` :

```
GAMP=CALC_CHAMP (reuse=GAMP,  
  RESULTAT=GAMP,  
  VARI_INTERNE=' VAEX_NOEU');
```

Since it is just a question of extracting one (and only one!!) variable intern, them `cham_elem` correspondents must be calculated as a preliminary:

```
U0=CALC_CHAMP (reuse =U0,  
  MODELE=MODELE,  
  CHAM_MATER=CHMAT0,  
  TOUT_ORDRE=' OUI',  
  VARI_INTERNE= ('VARI_ELNO'),  
  RESULTAT=U0,);
```

The list of the various reference symbols of the internal variables is:

"DPORO"	variation of the porosity of material
"DRHOLQ"	variation of the density of material
"DPVP"	variation of the steam pressure
"SATLIQ"	saturation of the liquid
"EVP"	cumulated voluminal plastic deformation
"IND_ETA"	Mechanical indicator of state
"D"	Value of the damage
"IND_END"	Indicator of damage
"TEMP_MAX"	Maximum temperature
"GAMP"	Plastic deformation déviatoire cumulated
"PCR"	Critical pressure
"SEUIL_HYD"	Hydrous threshold
"IND_HYD"	Hydrous indicator of irreversibility
"PCOHE"	Pressure of cohesion
"COMP_ROC"	Behavior of the rock
"SEUIL_ISO"	Isotropic threshold
"ANG_DEV"	Angle of the threshold déviatoire
"X11"	Components of the kinematic tensor of work hardening
"X22"	Components of the kinematic tensor of work hardening
"X33"	Components of the kinematic tensor of work hardening
"X12"	Components of the kinematic tensor of work hardening
"X13"	Components of the kinematic tensor of work hardening
"X23"	Components of the kinematic tensor of work hardening
"DIST_DEV"	Distance standardized with the threshold déviatoire
"DEV_SUR_CRIT"	Relationship between the threshold déviatoire and the critical threshold deviatoric
"DIST_ISO"	Distance standardized with the isotropic threshold
"NB_ITER"	Iteration count internal
"STOP"	Value of the local test of stop of the iterative process
"NB_REDE"	Number of local recutting of the step of time
"SIGN"	Sign of the contracted product of the deviatoric constraint by the deviatoric plastic deformation

## Note:

When the variable to be extracted is not part of the internal variables of the laws concerned, an alarm is emitted but the field is affected all the same with `R8VIDE ()`.

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## 2.6.3 Isovaleurs

Caution: linear distinction resolution and quadratic grid

One recalls that for any problem THM and in order to avoid any ambiguity for the user, the grid used is always quadratic. On the other hand the resolution of the hydraulic and thermal problem is linear: unknown factors *PRE1* , *PRE2* and *TEMP* thus exist only on the nodes tops of the grid.

At the conclusion of calculation, one gets a result in this form:

- Pressures *PRE1* , *PRE2* and temperatures *TEMP* are on the nodes tops of the elements.
- The internal variables, the constraints are on the points of gauss and/or the nodes of the quadratic grid (according to whether one into selective or in is lumpé) and displacements mechanical are on the tops and the nodes mediums.

There is thus a conflict between the quadratic grids and linear calculations what will pose a problem for example to trace isovaleurs.

There then exists a manner simple to be freed from this problem by projecting the whole of the results on the linear grid resulting from the quadratic grid. Thus all the results will be defined at the same place (on the tops).

For *TEMP* , *PRE1* and *PRE2* , it is enough to project as on the following example:

### ## projection of the quadratic grid on the linear grid:

```
MAILQ4 = CREA_MALLAGE (
    GRID = E-MAIL,
    QUAD_LINE = _F (ALL = 'YES'),
)
```

### ## assignment of the model corresponding:

```
MODELQ4=AFFE_MODELE (MALLAGE=MAILQ4,
    AFFE=_F (TOUT=' OUI ',
    PHENOMENE=' MECANIQUE ',
    MODELISATION=' D_PLAN',),),);
```

### ## projection of the result on this new model:

```
RESULIN = PROJ_CHAMP (
    METHODE=' ELEM ',
    RESULTAT=resu,
    MODELE_1=MODELQ8,
    MODELE_2=MODELQ4,
    NOM_CHAM = ' DEPL ',
    TOUT_ORDRE=' OUI ')
```

### ## usual postprocessing but on the linear grid:

```
IMPR_RESU (FORMAT=' MED ',
    RESU=_F (
    RESULTAT=RESULIN,
    NUME_ORDRE= (1,10,20),
    NOM_CMP = ('PRE1', 'PRE2',),
    MALLAGE=MAILQ4,),);
```

There exists an alternative method, which can prove faster for the large industrial studies. This method uses `MACR_ADAP_MAIL`. It is supposed that `resu` is composed of `nbinst` moments stored in the list `linst`. Preceding postprocessing can also be done in the following way:

```
PRE = [Nun] *nbinst;
PREB = [Nun] *nbinst;

for K in arranges (nbinst):

    PRE [K] =CRÉA_CHAMP (TYPE_CHAM=' NOEU_DEPL_R',
                        OPERATION=' EXTR',
                        RESULTAT=resu,
                        NOM_CHAM=' DEPL',
                        INST=linst [K],);

motcle1= {}
motcle2= {}

motcle1 ['MAJ_CHAM'] = []
motcle2 ['AFFE'] = []

for K in arranges (nbinst):

    PREB [K] =CO ('PREB_%d' % (K))

    motcle1 ['MAJ_CHAM'] .append (
        _F (TYPE_CHAM=' NOEU_DEPL_R', CHAM_GD = PRE [K],
            CHAM_MAJ = PREB [K],),);

    motcle2 ['AFFE'] .append (
        _F (CHAM_GD=PREB [K], INST=linst [K],),);

MACR_ADAP_MAIL (ADAPTATION=' MODIFICATION', DEGRE=' OUI',
                MAILLAGE_N = MAILQ8,
                MAILLAGE_NP1 = CO ('MAILQ4'),
                ** motcle1);

RESULINB=CRÉA_RESU (OPERATION=' AFFE', TYPE_RESU=' EVOL_NOLI', NOM_CHAM='
DEPL', ** motcle2);
```

## 2.7 Some cases tests

On a purely informative basis, one recapitulates here some cases tests available in the base of Code\_Aster. This list is absolutely not exhaustive but gives access directly a certain number of representative examples.

Name of CAS-test	Type of modeling THM	Phenomenon represented	Geometrical modeling	Mixing rate
Wtna109a	AXIS_THVD	Désaturation by heating of a medium without air	axisymmetric	LIQU_VAPE
Wtna110a	AXIS_HH2MS	Modeling of a swelling of a clay	axisymmetric	LIQU_AD_GAZ_VAPE
Wtna107	AXIS_THMS	Heating of a medium saturated (THM)	axisymmetric	LIQU_SATU
wtna112	AXIS_THMS	Thermal pressurization of a drained test-tube	axisymmetric	LIQU_SATU
Wtnp117a	D_PLAN_HHS	Capillary rebalancing of 2 materials	plane	LIQU_GAZ

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		(BO/BG)		
Wtnp118a	D_PLAN_HH2D	Gravitating rebalancing of a column	plane	LIQU_AD_GAZ_VAPE
Wtnp112d	D_PLAN_HMD	Resaturation of a column (assumption of Richards)	plane	LIQU_GAZ_ATM
Wtnp101a	D_PLAN_HM	Modeling of a medium saturated with gas	plane	GAS
Wtnl100a	D_PLAN_HMD D_PLAN_HM_SI	Problem of consolidation (Therzagi)	plane	LIQU_SATU
Wtnv123a	3D_HHM	Hydrostatic test then triaxial with suction fixes (model of Barcelona)	3D	LIQU_GAZ
Wtnp113a	D_PLAN_THHD	Resaturation of an cell by the solid mass	plane	LIQU_GAZ
Wtnv121a	3D_HHMD	Damping of the concrete with damage	3D	LIQU_GAZ
Wtnv130a	3D_THH2S	Heating of a porous environment with dissolved air	3D	LIQU_AD_GAZ_VAPE
wtnv140	3D_HMS	Anisotropic drained triaxial compression test	3D	LIQU_SATU

## 3 Modelings THM by an approach second gradient

Modelings of the type second gradient and second gradient of dilation are described in documentation [R5.04.03] within the framework as of porous environments. Their use is essential when the mechanical laws of behaviors model a degradation of material – one speaks about lenitive laws. Indeed, in this case, the solutions depend on the grid including when the medium is coupled with the equations of hydraulics.

The digital integration of these models followed an atypical protocol at the time of its implementation to facilitate its use in Code\_Aster. Thus, the regularizing part (second gradient) is defined as a patch that it is enough “to stick” on the structure to model. One described the stages below to be followed to produce such a simulation.

- 1) Definition of the patch
- 2) Choice of the model
- 3) Definition of material
- 4) Boundary conditions
- 5) Calculation

### 3.1 Definition of the patch

For the simulation of a study THM by an approach of the type second gradient, it is necessary to define a quadratic grid for the discretization of the structure, then a second grid for the regularizing patch. characteristic of this second grid is that it must necessarily be topologically identical to the first grid (same nodes and same geometric standards. For reasons of digital simplification and reasons of coherence of models, one advises to use the following procedure:

- 1) Definition of a space discretization for the structure and modeling THM;
- 2) Duplication of the preceding grid on the whole of the structure by the order CREA\_MALLAGE to define the patch
- 3) Possible modification of the type of meshes for a study with multipliers of Lagrange in the centers of the elements.

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## 3.1.1 Stage 1. Definition of the grid of the structure

This first stage is to be produced by a mailleur to discretize the structure. One recovers then the grid by the order *Code\_Aster* :

reading of the grid (quadratic)

```
MY = LIRE_MAILLAGE ( )
```

## 3.1.2 Stage 2. Duplication of the grid to define the patch

There exists in *Code\_Aster* a procedure which makes it possible to duplicate a grid by preserving the same nodes that the original grid – it is essential that the nodes of the first grid are included in the patch (cf [R5.04.03]). It is necessary to define this second grid to make it possible to define modeling second gradient in the regularizing patch.

Duplication of the grid (quadratic). Only the meshes are duplicated, the nodes remain common. The goal is to associate with each one of these grids a different modeling.

```
MAIL=CRÉA_MAILLAGE (GRID          = MY,  
                    CREA_GROUP_MA = ( _F (NAME          = 'ROCHE_REG',  
                                           GROUP_MA      = 'ROCK' ) ) )
```

## 3.1.3 Stage 3. Modification (possible) of the grid of the patch

There exist various discretizations finite elements to interpolate modelings second gradient (with or without multipliers of Lagrange, multipliers of Lagrange in the center of the elements or the nodes tops). Consequently it is necessary to adapt the grid of the patch to the space of discretization of modeling second gradient.

For example to take into account an interpolation with multipliers of Lagrange in the centers of the elements, it is necessary to define the nodes in the centers of the elements because those are not envisaged, in general, in the space discretizations suggested by most mailleurs. Thus in this case, one can use the order *Code\_Aster* following:

Introduction of central nodes to the finite elements of the new grid for an interpolation  $P2-P1-P0$ . Procedure necessary to take into account the interpolations of the multipliers of Lagrange.

```
MAYLLAGE=CRÉA_MAILLAGE (GRID      = E-MAIL,  
                        MODI_MAILLE = ( _F (GROUP_MA = 'ROCHE_REG',  
                                           OPTION   = 'QUAD8_9' ),  
                                          _F (GROUP_MA = 'ROCHE_REG',  
                                           OPTION   = 'TRIA6_7' ) ) )
```

This stage is not possible that in 2D when the interpolation finite element considers multipliers of constant Lagrange by element.

## 3.2 Choice of the model

The “patches regularizing” second gradient or second gradient of dilation are to be combined with any type of modeling THM. They have interest, of course, only in the presence of one mechanical component (lenitive). Modelings available are:

Modeling	Geometrical modeling	Phenomenon taken into account
D_PLAN_2DG	Plane	Second gradient
D_PLAN_DIL	Plane	Second gradient of dilation
3D_DIL	3D	Second gradient of dilation

### Note:

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*It should be noted that it is strongly advised to use modelings second gradient of dilation to treat the behaviors of the grounds and of the rocks or more particularly any type of material presenting a voluminal variation during its degradation .*

The nodal unknown factors of modelings THM are then enriched after addition by the "patch" second gradient. The number of unknown factors varies according to the patch considered and the type of meshes characterizing the space discretization of the patch. For modeling second gradient of dilation it is thus by the choice of the topology of the mesh that the interpolation of the multipliers of Lagrange will be given (see the table below). One summarizes in the table below the various possibilities where one notes in agreement with [R5.04.03],  $f_{ij}$  components of the tensor of the microscopic deformations,  $\chi$  microscopic voluminal deformation and  $\lambda$  the multiplier of Lagrange:

Modeling	Type of meshes	Degrees of freedom	Position of the degree of freedom
D_PLAN_2DG	TRIA7, QUAD9	$f_{ij}$	At the tops of each element
		$\lambda_{ij}$	In the center of each element
D_PLAN_DIL	TRIA7, QUAD9	$\chi$	At the tops of each element
		$\lambda$	In the center of each element
	TRIA6, QUAD8	$\chi$	At the tops of each element
3D_DIL	TETRA10, HEXA20, PENTA15	$\chi, \lambda$	At the tops of each element

One proceeds then in the following way:

```
MODEL = AFFE_MODELE (GRID = GRID,
                    AFFE      = (_F (GROUP_MA      = 'ROCK',
                                    PHENOMENON    = 'MECHANICAL',
                                    MODELING      = 'D_PLAN_HMS'),
                                _F (GROUP_MA      = 'ROCHE_REG',
                                    PHENOMENON    = 'MECHANICAL',
                                    MODELING      = 'D_PLAN_DIL'))))
```

### 3.3 Definition of material

It is necessary, besides the definition of the parameters materials necessary for calculation THM describes in the preceding chapter, to add a parameter which characterizes the length characteristic of modeling second gradient (cf [R5.04.03]). This data characterizes in fact the dimension of the vicinity which contributes to the description of a material point.

This length is defined starting from the components material  $A1$  and  $A3$  law of linear behavior of elasticity second gradient inspired by work of Mindlin in the case of modeling second gradient of dilation. It is in the determination of these parameters that the greatest difficulty resides. There does not exist today of analytical method to identify them. The practice is to carry out some tests precondition. In the case of modelings second gradient this length is function of the 5 components  $A1$ ,  $A2$ ,  $A3$ ,  $A4$  and  $A5$ , to inform under the keyword ELAS\_2NDG of DEFI\_MATERIAU (cf [R5.04.03]).

One can, moreover, to add a digital parameter of penalization. It was shown that the term of penalization of modelings second gradient of dilation improves digital convergence without disturbing the quality of the results.

Here an example of definition of the parameters material for the part second gradient.

```
SOL2 = DEFI_MATERIAU (ELAS_2NDG = _F (A1 = 4.0E4,
                                       A2 = 0.0,
                                       A3 = 0.0,
                                       A4 = 0.0,
                                       A5 = 0.0),
                    NON_LOCAL = _F (PENA_LAGR=1.0E12, , ,));
```



Then assignment of the parameters materials according to the same procedure as for the definition of modelings.

```
= AFFE_MATERIAU (GRID SUBDUE = GRID,  
                 AFFE      = (_F (ALL      = 'ROCK',  
                                MATER    = SOL_HM,)),  
                 _F (GROUP_MA = 'ROCHE_REG',  
                    MATER    = SOL2)))
```

## 3.4 Impact on the boundary conditions

There is no impact to bring in the command file Code\_Aster to take into account the boundary conditions with modelings second gradient compared to classical modelings THM. On the other hand, it is essential to note that the physical significance of the boundary conditions of pressure of normal constraints is modified with modelings second gradient (cf [R5.04.03]).

## 3.5 Resolution DU problem

Calculation is to be carried out by the order `STAT_NON_LINE`. It is enough to add to classical calculation THM the relation of behavior of elasticity second gradient on the grid corresponds to the patch as on the example below (keyword `ELAS`). There is no incompatibility with the laws of behavior. To note, all the same, that a simulation THM by an approach second gradient has interest only in the presence of one mechanical component in coupled calculation.

It is important to note that when modeling takes into account an interpolation of the constant multipliers of Lagrange by elements it is necessary to use the solver Mumps for the resolution.

Definition of nonlinear static calculation with a law of behavior associated with each one of modeling: behavior of the Drucker-Prager type for the first gradient, and linear elasticity for the second gradient

```
U1 = STAT_NON_LINE (MODEL      = MODEL,  
                   CHAM_MATER = SUBDUE,  
                   EXCIT      = (_F (LOAD = CHCI),...),  
                   SOLVEUR    = (_F (METHODE=' MUMPS',)),  
                   BEHAVIOR    = (_F (GROUP_MA=' ROCHE',  
                                     RELATION = 'DRUCK_PRAGER',)),  
                               _F (GROUP_MA = 'ROCHE_REG',  
                                   RELATION = 'ELAS',)),),  
                   NEWTON     = _F (MATRIX = 'TANGENT', REAC_ITER = 1),  
                   INCREMENT = _F (LIST_INST = TIME))
```

One will find an example of modeling by second gradient, for example in the case test `ss11117`.

## Annexe 1 Generalized constraints and internal variables

Constraints:

Number	Name of component Aster	Contents	Modelings
1	SIXX	$\sigma'_{xx}$	So mechanical (. M ...)
2	SIYY	$\sigma'_{yy}$	So mechanical (. M ...)
3	SIZZ	$\sigma'_{zz}$	So mechanical (. M ...)
4	SIXY	$\sigma'_{xy}$	So mechanical (. M ...)
5	SIXZ	$\sigma'_{xz}$	So mechanical (. M ...)
6	SIYZ	$\sigma'_{yz}$	So mechanical (. M ...)
7	SIPXX	$\sigma_{p_{xx}}$	So mechanical (. M ...)
8	SIPYY	$\sigma_{p_{yy}}$	So mechanical (. M ...)
9	SIPZZ	$\sigma_{p_{zz}}$	So mechanical (. M ...)
10	SIPXY	$\sigma_{p_{xy}}$	So mechanical (. M ...)
11	SIPXZ	$\sigma_{p_{xz}}$	So mechanical (. M ...)
12	SIPYZ	$\sigma_{p_{yz}}$	So mechanical (. M ...)
13	M11	$m_w$	In all the cases
14	FH11X	$M_{w_x}$	In all the cases
15	FH11Y	$M_{w_y}$	In all the cases
16	FH11Z	$M_{w_z}$	In all the cases
17	ENT11	$h_w^m$	In all the cases with thermics
18	M12	$m_{vp}$	If 2 unknown pressures (. HH ...)
19	FH12X	$M_{vp_x}$	If 2 unknown pressures (. HH ...)
20	FH12Y	$M_{vp_y}$	If 2 unknown pressures (. HH ...)
21	FH12Z	$M_{vp_z}$	If 2 unknown pressures (. HH ...)
22	ENT12	$h_{vp}^m$	If 2 unknown pressures and thermics (. THH ...)
23	M21	$m_{as}$	If 2 unknown pressures (. HH ...)
24	FH21X	$M_{as_x}$	If 2 unknown pressures (. HH ...)
25	FH21Y	$M_{as_y}$	If 2 unknown pressures (. HH ...)
26	FH21Z	$M_{as_z}$	If 2 unknown pressures (. HH ...)
27	ENT21	$h_{as}^m$	If 2 unknown pressures and thermics (. THH ...)
28	M22	$m_{ad}$	If modeling of the dissolved air (...HH2...)
29	FH22X	$M_{ad_x}$	If modeling of the dissolved air (...HH2...)
30	FH22Y	$M_{ad_y}$	If modeling of the dissolved air (...HH2...)

31	FH22Z	$M_{ad_z}$	If modeling of the dissolved air (...HH2...)
32	ENT22	$h_{ad}^m$	If modeling of the dissolved and thermal air (... T <sub>HH2</sub> ...)
33	QPRIM	$Q'$	So thermal
34	FHTX	$q_x$	So thermal
35	FHTY	$q_y$	So thermal
36	FHTZ	$q_z$	So thermal

In the case without mechanics, and for the laws of behaviors (LIQU\_VAPE\_GAZ, LIQU\_VAPE, LIQU\_AD\_GAZ\_VAPE, 'LIQU\_AD\_GAZ') the internal variables are:

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

In the case without mechanics, and for the laws of behaviors (LIQU\_GAZ, LIQU\_GAZ\_ATM,) the internal variables are:

Number	Name of 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 of 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 Additional elements on the boundary conditions in THM

In what follows one does not take into account the dissolved air (the index  $lq$  corresponds then to that of water  $w$ ) and one sticks to the case unsaturated.

We point out here the choice of the unknown factors of pressure.

Behavior	LIQU_GAZ and LIQU_VAPE_GAZ
PRE1	Capillary pressure: $p_c = p_{gz} - p_{lq}$
PRE2	Gas pressure $p_{gz} = p_{vp} + p_{as}$

### A2.1 Variational formulation of the conservation equations

One refers here to [R7.01.11]. These equations are

$$\dot{m}_{lq} + \dot{m}_{vp} + Div(M_{lq} + M_{vp}) = 0 \quad \text{éq A5.1-1}$$

$$\dot{m}_{as} + Div(M_{as}) = 0 \quad \text{éq A5.1-2}$$

The deduced variational formulation is given by

$$-\int_{\Omega} (\dot{m}_{lq} + \dot{m}_{vp}) \pi_1 d\Omega + \int_{\Omega} (M_{lq} + M_{vp}) \cdot \nabla \pi_1 d\Omega = \int_{\partial\Omega} (M_{lq_{ext}} + M_{vp_{ext}}) \cdot \pi_1 d\Gamma \quad \forall \pi_1 \in P_{1_{ad}} \quad \text{éq A5.1-3}$$

$$-\int_{\Omega} \dot{m}_{as} \pi_2 d\Omega + \int_{\Omega} M_{as} \cdot \nabla \pi_2 d\Omega = \int_{\partial\Omega} M_{as_{ext}} \cdot \pi_2 d\Gamma \quad \forall \pi_2 \in P_{2_{ad}} \quad \text{éq A5.1-4}$$

The capillary pressures and of gas are related to the pressure of water, vapor and dry air by the relations:

$$p_c = p_{gz} - p_{lq} \quad \text{éq A5.1-5}$$

$$p_{gz} = p_{vp} + p_{as} \quad \text{éq A5.1-6}$$

The steam pressure is not an independent variable. It is connected to the pressure of liquid  $p_{lq}$  by the relations

$$\frac{dp_{vp}}{\rho_{vp}} = \frac{dp_{lq}}{\rho_{lq}} + (h_{vp}^m - h_{lq}^m) \frac{dT}{T} \quad \text{éq A5.1-7}$$

$$dh_{lq}^m = C_{lq}^p dT + (1 - 3\alpha_{lq} T) \frac{dp_{lq}}{\rho_{lq}} \quad \text{éq A5.1-8}$$

$$dh_{vp}^m = C_{vp}^p dT \quad \text{éq A5.1-9}$$

These relations show that the steam pressure is given completion not the knowledge of  $p_{lq}$  (and of its

evolution). Often, these relations are used to establish the law of Kelvin,  $\frac{p_{lq} - p_{lq}^0}{\rho_{lq}} = \frac{R}{M_{vp}^{ol}} T \ln\left(\frac{p_{vp}}{p_{vp}^{sat}(T)}\right)$ , but

this law is not used directly in Aster.

The reference documents Aster do not say anything on what are the variables  $\pi_1$  and  $\pi_2$ . But two elements can put to us on the track:

- On the one hand,  $\pi_1 \in P_{1_{ad}}$  and  $\pi_2 \in P_{2_{ad}}$  whereas  $P_{1_{ad}}$  and  $P_{2_{ad}}$  are spaces of membership of  $PRE1$  and  $PRE2$  (thus including their boundary conditions).
- In addition, in chapter 7. of [R7.01.10], one sees that the virtual deformation  $E_g^{*el} = (v, \varepsilon(v), \pi_1, \nabla \pi_1, \pi_2, \nabla \pi_2, \tau, \nabla \tau)$  is related to the vector of virtual displacement nodal  $U^{*el} = (v, \pi_1, \pi_2, \tau)$  by the same operator  $Q_g^{el}$  that which connects between them the deformation  $E_g^{el} = (u, \varepsilon(u), p_1, \nabla p_1, p_2, \nabla p_2, T, \nabla T)$  and nodal displacement  $U^{el} = (u, p_1, p_2, T)$  :
  - $E_g^{*el} = Q_g^{el} U^{*el}$
  - $E_g^{el} = Q_g^{el} U^{el}$

It is then clear that  $\pi_1$  and  $\pi_2$  are virtual variations of  $p_1$  and  $p_2$   
From where the table:

$$\begin{aligned} p_1 = p_c &\Rightarrow \pi_1 = \delta p_c = p_c^* \\ p_1 = p_{lq} &\Rightarrow \pi_1 = \delta p_{lq} = p_{lq}^* \\ p_2 = p_{gz} &\Rightarrow \pi_2 = \delta p_{gz} = p_{gz}^* \end{aligned}$$

## A2.2 Case of boundary conditions utilizing principal unknown factors

What we say in this paragraph and the following is relative to part of the border  $\partial\Omega_d$  on which conditions are prescribed: nothing prevents of course that these conditions are not the same ones on parts of different borders. We treat in this chapter the usual case where one imposes conditions on  $PRE1$  and/or  $PRE2$ , in opposition to the following chapter where we will speak about linear relations between unknown factors.

$$\begin{aligned} p_c &= p_{gz} - p_{lq} = p_c^{imp} \\ p_{gz} &= p_{as} + p_{vp} = p_g^{imp} \end{aligned}$$

Flows are then computation results by [éq A5.1-3] and [éq A5.1-4]

- **Dirichlet  $PRE1$ , Neuman  $PRE2$**

It is the case where one imposes a value on  $PRE1$  and a value with flow associated with  $PRE2$ , by not saying anything on  $PRE2$  or by giving a value to `FLUN_HYDR2` of `FLUX_THM_REP` in `AFPE_CHAR_MECA`. Let us call  $M_{2_{ext}}$  this imposed quantity, which will be worth 0 if nothing is known as compared to  $PRE2$ . We will note  $p_1 = p_1^{imp}$  the condition imposed on  $PRE1$

This corresponds to:

$$\begin{aligned} p_c &= p_{gz} - p_{lq} = p_c^{imp} \\ p_1^{imp} &= p_c^{imp} \end{aligned}$$

To make the demonstration within the nonhomogeneous framework, it would be necessary to introduce a raising of the condition  $p_1 = p_1^{imp}$  (i.e. a particular field checking this condition). That weighs down the writings and does not bring anything, one thus places itself within the homogeneous framework  $p_1^{imp} = 0$

In [éq A5.1-3] and [éq A5.1-4], one can thus take and  $\pi_2$  unspecified and  $\pi_1$  checking  $\pi_1 = 0$  on  $\partial\Omega_d$ . One then starts to take  $\pi_1 = 0$  and  $\pi_2 = 0$  on all the edge  $\partial\Omega$  and one obtains [éq A5.1-1] and [éq A5.1-2] within

the meaning of the distributions. One multiplies [éq A5.1- then1] by  $\pi_1$  such as  $\pi_1=0$  on  $\partial\Omega_d$  one multiplies [éq A5.1-2] by  $\pi_2$  unspecified, one integrates by part, one takes account of [éq A5.1-3] and [éq A5.1-4] and one obtains, while indicating by  $n$  the normal at the edge:

$$\int_{\partial\Omega_d} M_{as} \cdot n \cdot \pi_2 d\Gamma = \int_{\partial\Omega_d} M_{2ext} \pi_2 d\Gamma, \quad \forall \pi_2$$

One from of deduced

$$M_{as} \cdot n = M_{2ext} \text{ sur } \partial\Omega_d$$

- **Dirichlet PRE2 , Neuman PRE1**

It is the case where one imposes a value on PRE2 and a value with flow associated with PRE1 , by not saying anything on PRE1 or by giving a value to FLUN\_HYDR1 of FLUX\_THM\_REP in AFFE\_CHAR\_MECA. Let us call  $M_{1ext}$  this imposed quantity, which will be worth 0 if nothing is known as compared to PRE2 . We will note  $p_2 = p_2^{imp}$  the condition imposed on PRE2 .

This corresponds to:

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

$$p_2^{imp} = p_{gz}^{imp}$$

The demonstration is the same one as in the preceding paragraph and leads to:

$$(M_{lq} + M_{vp}) \cdot n = M_{1ext} \text{ sur } \partial\Omega_d$$

## A5.3 Case of boundary conditions utilizing linear relations between principal unknown factors

Code\_Aster allows to introduce like boundary conditions of the relations between degrees of freedom, carried by the same node or by different nodes. This possibility is reached via the keyword LIAISON\_DDL order AFFE\_CHAR\_MECA.

That is to say  $p_{lq}^{imp}$  the value which one wants to impose on the pressure of liquid on  $\partial\Omega_d$  . Taking into account [éq A5.1-5], and choice of the principal unknown factors for this behavior, one writes:

$$p_{gz} - p_c = p_2 - p_1 = p_{lq}^{imp} \quad \text{éq A5.3-1}$$

The linear relations are treated in Aster by introduction of multipliers of Lagrange. This corresponds in the species to the following formulation:

To find  $p_1, p_2, \mu$  such as:

$$-\int_{\Omega} (m_{lq} + m_{vp}) \pi_1 d\Omega + \int_{\Omega} (M_{lq} + M_{vp}) \cdot \nabla \pi_1 d\Omega - \int_{\Omega} m_{as} \pi_2 d\Omega + \int_{\Omega} M_{as} \cdot \nabla \pi_2 d\Omega +$$

$$+ \int_{\partial\Omega_d} \mu^* (p_2 - p_1 - p_{lq}^{imp}) d\Gamma + \int_{\partial\Omega_d} \mu (\pi_2 - \pi_1 - p_{lq}^{imp}) d\Gamma \quad \forall \pi_1, \pi_2, \mu^* \quad \text{éq A5.3-2}$$

To make the demonstration within the nonhomogeneous framework, it would be necessary to introduce a raising of the condition  $p_2 - p_1 - p_{lq}^{imp} = 0$  (I.e. of the particular fields checking this condition). That weighs

down the writings and does not bring anything, one thus places itself within the homogeneous framework  $p_{lq}^{imp} = 0$ .

One then starts to take  $\pi_1 = 0$  and  $\pi_2 = 0$  on all the edge  $\partial \Omega$  and one obtains [éq A5.1-1] and [éq A5.1-2] within the meaning of the distributions. One multiplies then [éq A5.1-1] by  $\pi_1$  unspecified one multiplies [éq A5.1-2] by  $\pi_2$  unspecified, one integrates by part, one carries the results found in [éq A5.3-2] and one obtains:

$$\int_{\partial \Omega_d} (M_{lq} + M_{vp}) \cdot n \cdot \pi_1 d\Gamma + \int_{\partial \Omega_d} M_{as} \cdot n \cdot \pi_2 d\Gamma + \int_{\partial \Omega_d} \mu^* (p_2 - p_1) d\Gamma + \int_{\partial \Omega_d} \mu (\pi_2 - \pi_1) d\Gamma = 0 \quad \forall \pi_1, \pi_2, \mu^* \quad \text{éq A5.3-3}$$

It is clear that [éq A5.3-3] gives again well  $p_2 - p_1 = p_{lq}^{imp} = 0$

While taking moreover  $\pi_2 - \pi_1 = 0$ , one finds:

$$\int_{\partial \Omega_d} (M_{lq} + M_{vp} + M_{as}) \cdot n \cdot \pi_1 d\Gamma = 0 \quad \forall \Gamma_1$$

From where one deduces:

$$(M_{lq} + M_{vp} + M_{as}) \cdot n = 0 \text{ sur } \partial \Omega_d \quad \text{éq A5.3-4}$$

## A5.4 Nonlinear cases

We do not make here that to tackle more difficult questions consisting in imposing either the steam pressure or the air pressure dryness. Taking into account the relations [éq A5.1-7], [éq A5.1-8] and [éq A5.1-9] to impose a value on the steam pressure amounts imposing a nonlinear relation on the pressure of liquid; just as to impose an air pressure dryness on the gas pressure.

As example, we approach the case of an air pressure dryness imposed for a behavior LIQU\_VAPE\_GAZ, and we suppose that we know to write the nonlinear relation connecting the steam pressure and the pressure of liquid.

The relation to be imposed is thus:

$$p_{as} = p_{gz} - p_{vp} = p_2 - p_{vp} = p_{as}^{imp} \quad \text{éq A5.4-1}$$

By differentiating this relation, one will find a condition on the virtual variations of pressures:

$$dp_{as} = dp_{gz} - \frac{\partial p_{vp}}{\partial p_{lq}} dp_{lq} = dp_{gz} - \frac{\partial p_{vp}}{\partial p_{lq}} (dp_{gz} - dp_c)$$

That is to say still

$$dp_{as} = dp_2 - \frac{\partial p_{vp}}{\partial p_{lq}} (dp_2 - dp_1) = \frac{\partial p_{vp}}{\partial p_{lq}} dp_1 + \left(1 - \frac{\partial p_{vp}}{\partial p_{lq}}\right) dp_2$$

The variational formulation would be then:

$$-\int_{\Omega} (\dot{m}_{lq} + \dot{m}_{vp}) \pi_1 d\Omega + \int_{\Omega} (M_{lq} + M_{vp}) \cdot \nabla \pi_1 d\Omega - \int_{\Omega} m_{as} \pi_2 d\Omega + \int_{\Omega} M_{as} \cdot \nabla \pi_2 d\Omega + \int_{\partial \Omega_d} \mu^* (p_2 - p_{vp} - p_{as}^{imp}) d\Gamma + \int_{\partial \Omega_d} \mu \left( \frac{\partial p_{vp}}{\partial p_{lq}} \pi_1 + \left(1 - \frac{\partial p_{vp}}{\partial p_{lq}}\right) \pi_2 \right) d\Gamma \quad \forall \pi_1, \pi_2, \mu^*$$

And one would find:

$$\int_{\partial\Omega_d} (M_{lq} + M_{vp}) \cdot n \cdot \pi_1 d\Gamma + \int_{\partial\Omega_d} M_{as} \cdot n \cdot \pi_2 d\Gamma + \int_{\partial\Omega_d} \mu \left( \frac{\partial p_{vp}}{\partial p_{lq}} \pi_1 + \left( 1 - \frac{\partial p_{vp}}{\partial p_{lq}} \right) \pi_2 \right) d\Gamma = 0 \quad \forall \pi_1, \pi_2$$

While taking  $\frac{\partial p_{vp}}{\partial p_{lq}} \pi_1 + \left( 1 - \frac{\partial p_{vp}}{\partial p_{lq}} \right) \pi_2 = 0$  one would find:

$$\left( 1 - \frac{\partial p_{vp}}{\partial p_{lq}} \right) (M_{lq} + M_{vp}) \cdot n - \frac{\partial p_{vp}}{\partial p_{lq}} M_{as} \cdot n = 0 \quad \text{éq A5.4-2}$$