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Note of use of model THM

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.

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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 $P1$ 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.

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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)

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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)

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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).

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

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	$PRE1^{ddl}$	$PRE2^{ddl}$	T^{ddl}
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	

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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,
```

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```
                                        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 $P/\rho = RT/Mv$ where P is the pressure, ρ density, Mv 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.

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/ `'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_SATU	LIQU_GAZ	GAS	LIQU_GAZ_ATM	LIQU_VAPE_GAZ	LIQU_AD_GAZ_VAPE	LIQU_AD_GAZ	LIQU_VAPE
THM_INIT	*O*	*O*	*O*	*O*	*O*	*O*	*O*	*O*
PRE1	F	F	F	F	F	F	F	F
PRE2		F			F	F	F	
PORO	O	O	O	O	O	O	O	O
TEMP	F	F	F	F	F	F	F	F
PRES_VAPE					O	O	O	O
THM_DIFFU	*O*	*O*	*O*	*O*	*O*	*O*	*O*	*O*
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
If law HYDR_UTIL (cf chapter 2.5) :								
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_SATU				O	O	O	O	O
PERM_GAZ					O	O	O	O
D_PERM_SATU_GAZ					O	O	O	O
D_PERM_PRES_GAZ					O	O	O	O
If law HYDR_VGM or HYDR_VGC (cf chapter 2.5) :								
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	
FICKA_PA						F	F	
FICKA_PL						F	F	
FICKA_S						F	F	
D_FA_T						F	F	
CP	T	T	T	T	T	T	T	T
PERM_IN/PERM_END/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								

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LAMB_CT/LAMB_C_L, LAMB_C_N, LAMB_C_T							
D_LB_T/D_LB_TOUT, D_LB_TL, D_LB_T,							
D_LB_S							
D_LB_PHI							
THM_LIQU	O	O	O	O	O	O	O
RHO	O	O	O	O	O	O	O
UN_SUR_K	O	O	O	O	O	O	O
VISC	O	O	O	O	O	O	O
D_VISC_TEMP	O	O	O	O	O	O	O
ALPHA	T	T	T	T	T	T	T
CP	T	T	T	T	T	T	T
THM_GAZ	O	O	O	O	O	O	
MASS_MOL	O	O	O	O	O	O	
VISC	O	O	O	O	O	O	
D_VISC_TEMP	O	O	O	O	O	O	
CP	T	T	T	T	T	T	
THM_VAPE_GAZ				O	O		O
MASS_MOL				O	O		O
CP				O	O		O
VISC				O	O		O
D_VISC_TEMP				O	O		O
THM_AIR_DISS					O	O	
CP					O	O	
COEF_HENRY					O	O	

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

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]
```

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)

Under this keyword, there are three sizes corresponding to degrees of freedom. For understanding these data well, it is necessary then to distinguish the unknown factors with the nodes, which we call $[u]^{ddl}$ and values defined under the keyword THM_INIT that us appelonS p^{ref} and T^{ref}

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

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 $\dfrac{p}{\rho} = \dfrac{R}{M} T$ for perfect gases, $\dfrac{d\rho_l}{\rho_l} = \dfrac{dp_l}{K_l} - 3\alpha_l dT$ for the liquid and in the relation capillary saturation/pressure.

One can thus choose to initialize the nodal values in THM_INIT (by defaults these values are worthless) or by the keyword ETAT_INIT order STAT_NON_LINE (cf 2.3) or by a combination of both (that can allow an easy conversion of Kelvin into degree for example).

◊   TEMP

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Temperature of reference T_{ref}. By default it is taken equalizes to zero. Attention the value of the temperature **initial** $T = T^{ddl} + T^{ref}$ must be strictly higher than zero.

◊   PRE1

By default it is taken equalizes to zero. 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 pressure **initial** gas $p = p^{ddl} + p^{ref}$ 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

By default it is taken equalizes to zero. For the behaviors LIQU_VAPE_GAZ, LIQU_AD_GAZ, LIQU_AD_GAZ_VAPE and LIQU_GAZ standard gas pressure. pressure **initial** gas $p = p^{ddl} + p^{ref}$ 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 hygroscopy. The relative humidity is the relationship between the steam pressure and the steam pressure saturating at the temperature considered. One then uses the law of Kelvin which gives the pressure of the liquid according to the steam pressure, of the temperature and of saturating steam pressure: $\dfrac{p_w - p_w^{ref}}{\rho_w} = \dfrac{R}{M_{vp}^{ol}} T \ln\left(\dfrac{p_{vp}}{p_{vp}^{sat}(T)}\right)$. *This relation is valid only for isothermal evolutions. It is stressed that* p_w^{ref} *corresponds in a state of 'balance to which corresponds* p_{pv}^{sat}, *this state of balance corresponds in fact to* $p_w^0 = p_{gz}^0 = 1\,atm$. *For evolutions with temperature variation, knowing a law giving the steam pressure saturating to the temperature* T_0 , *for example:* $p_{pv}^{sat}(T_0) = 10^{\left(2.7858 + \frac{T_0 - 273.5}{31.559 + 0.1354(T_0 - 273.5)}\right)}$
, *and a degree of hygroscopy* HR , *one from of deduced the steam pressure thanks to* $p_{pv}(T_0) = HR\,p_{pv}^{sat}(T_0)$.
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]
```

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```
                        ♦   UN_SUR_K        = usk  ,      [R]
                        ♦   VISC            = VI   ,      [function **]
                        ♦   D_VISC_TEMP     = dvi  ,      [function **]
                        ◊   ALPHA           = alp  ,      [R]
                        ◊   CP              = CP   ,      [R]
                        )
```

♦   RHO

Density initial liquidE.

♦   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 α_l

If p_l indicate the pressure of the liquid, ρ_l its density and T the temperature, the behavior of

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

◊   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, ρ_{gs} its density, R the constant of perfect gases and T

the temperature, the reaction of dry gas is: $\dfrac{p_{gs}}{\rho_{gs}} = \dfrac{RT}{M_{gs}}$.

♦   CP

Specific heat with constant pressure of dry gas.

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♦ 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:

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The constant of Henry that we use here expresses in $Pa.m^3.mol^{-1}$. 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 $\omega_l^a = \dfrac{P_{as}}{H}\dfrac{M_{as}^{ol}}{M_w}\rho_w$ with the concentration of air in the water which one can bring back to a density such as $\omega_l^a = \rho_{ad}$. H is a coefficient which is expressed in Pa . It will be necessary in these cases to write equivalence $K_H = H\dfrac{M_w}{\rho_w}$

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]
```

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```
                ◊   PERM_LIQU        = perml,        [function]
                ◊   D_PERM_LIQU_SATU = dperm,        [function]
                ◊   PERM_GAZ         = permg,        [function]
                ◊   D_PERM_SATU_GAZ  = dpsg ,        [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        = /   fvpg ,          [function]
                          / 1       ,         [DEFECT]
    ◊   FICKV_S         = /   fvs ,           [function]
                          / 1       ,         [DEFECT]
    ◊   D_FV_T          = /   dfvt ,          [function]
                          / 0       ,         [DEFECT]
    ◊   D_FV_PG         = /   dfvgp ,         [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    = /   lambtl ,     [function]
                      / 0             [DEFECT]
        |LAMB_TL    = /   lambtn ,     [function]
                      / 0             [DEFECT]
       /|LAMB_TOUT  = /   lambtl ,     [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       = /   lambctl,     [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          = /   dlambs ,         [function]
                          / 0       ,         [DEFECT]
    ◊  /D_LB_T          = /   dlambt ,         [function]
                          / 0       ,         [DEFECT]
```

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```
              /|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 " ρC_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.

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

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

viscosity, ρ_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 orthotropism. 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 **]

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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 Pr 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 Sr 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_PENTR   [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_e of pressure of entry of the law of Mualem Van-Genuchten. Medium désature only when the capillary pressure is higher than this value (0 by default).

◊   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 bracket 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 **]

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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 **]

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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:

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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	ρ_{lq}^0
♦	UN_SUR_K	$\dfrac{1}{K_{lq}}$
◊	ALPHA	α_{lq}
◊	CP	C_{lq}^p
♦	VISC	$\mu_{lq}(T)$
♦	D_VISC_TEMP	$\dfrac{\partial \mu_{lq}(T)}{\partial T}$

Keyword factor THM_GAZ

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

Keyword factor THM_VAPE_GAZ

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

Keyword factor THM_AIR_DISS

♦	CP	C_{ad}^p
♦	COEF_HENRY	K_H

Keyword factor THM_INIT

◊	TEMP	^{init}T

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◊	PRE1	$^{init}P_1$
◊	PRE2	$^{init}P_2$
♦	PORO	ϕ^0
◊	NEAR_VAPE	p_{vp}^0

•**Keyword factor THM_DIFFU**

◊	R_GAZ	R
♦	RHO	r_0
◊	CP	C_σ^s
◊	BIOT_COEF	b
◊	BIOT_L	b_L
◊	BIOT_N	b_N
◊	BIOT_T	b_T
◊	SATU_PRES	$S_{lq}(p_c)$
◊	D_SATU_PRES	$\dfrac{\partial S_{lq}(p_c)}{\partial p_c}$
♦	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	$\dfrac{\partial k_{lq}^{rel}(S_{lq})}{\partial S_{lq}}$
◊	PERM_GAZ	$k_{gz}^{rel}(S_{lq}, p_{gz})$
◊	D_PERM_SATU_GAZ	$\dfrac{\partial k_{gz}^{rel}(S_{lq}, p_{gz})}{\partial S_{lq}}$
◊	D_PERM_PRES_GAZ	$\dfrac{\partial k_{gz}^{rel}(S_{lq}, p_{gz})}{\partial p_{gz}}$
◊	FICKV_T	$f_{vp}^T(T)$
◊	FICKV_S	$f_{vp}^S(S)$
◊	FICKV_PG	$f_{vp}^{gz}(P_g)$
◊	FICKV_PV	$f_{vp}^{vp}(P_{vp})$

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◊	D_FV_T	$\dfrac{\partial f_{vp}^{T}(T}{\partial T}$
◊	D_FV_PG	$\dfrac{\partial f_{vp}^{gz}(P_{gz}}{\partial P_{gz}}$
◊	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	$\dfrac{\partial f_{ad}^{T}(T}{\partial T}$
◊	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	$\dfrac{\partial \lambda_{T}^{T}(T)}{\partial T}$
◊	D_LB_TL	$\dfrac{\partial \lambda_{T}^{T}(T)}{\partial T}$ according to L
◊	D_LB_TN	$\dfrac{\partial \lambda_{T}^{T}(T)}{\partial T}$ according to NR
◊	D_LB_TT	$\dfrac{\partial \lambda_{T}^{T}(T)}{\partial T}$ according to T (2D)
◊	LAMB_PHI	$\lambda_{\varphi}^{T}(\varphi)$
◊	D_LB_PHI	$\dfrac{\partial \lambda_{\varphi}^{T}(\phi)}{\partial \phi}$
◊	LAMB_S	$\lambda_{S}^{T}(S)$
◊	D_LB_S	$\dfrac{\partial \lambda_{S}^{T}(S)}{\partial S}$
◊	LAMB_CT	λ_{CT}^{T}
◊	LAMB_C_L	λ_{CT}^{T} according to L
◊	LAMB_C_N	λ_{CT}^{T} according to NR
◊	LAMB_C_T	λ_{CT}^{T} according to T (2D)

Note:

If there is thermics:
λ^{T} *is function of porosity, saturation and temperature and is given in the shape of the product of three functions:*

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

For the coefficient of Fick of the gas mixture, in the case `LIQU_VAPE_GAZ` and `LIQU_AD_GAZ_VAPE` $F_{vp}(P_{vp}, P_{gz}, T, S) = f^{vp}_{vp}(P_{vp}) . f^{gz}_{vp}(P_{gz}) . f^T_{vp}(T) . f^S_{vp}(S)$ with $f^T_{vp}(T)$ obligatory, other functions being taken by default equal to one, and the 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: $F_{ad}(P_{ad}, P_{lq}, T, S) = f^{ad}_{ad}(P_{ad}) . f^{lq}_{ad}(P_{lq}) . f^T_{ad}(T) . f^S_{ad}(S)$, with $f^T_{ad}(T)$ obligatory, other functions being taken by default equal to one, and the derivative equalizes to zero. One considers only the derivative compared to the temperature (the others are in any case taken equal to zero).

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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` , values are defined initial for porosity and the steam pressure (when it model account of the vapor takes) but too if it is wished 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. (the physical values of initializations will be the sum of the values defined under `THM_INIT` and under `ETAT_INIT`).**
- **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):

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

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. 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 enthali, 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 enthali. In practice, one can reason by considering that one has three states for the fluids:

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

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

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

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

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

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

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

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

Components of the tensor σ_p are calculated according to the water pressures. The adopted writing is incremental and, if it is wanted that valueS components of σ_p are coherent with Lbe valueS initial of pressures definedS underS wordSkeyS THM_INIT and ETAT_INIT, it is necessary to initialize the components of σ_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',
```

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```
                        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.),),),),);
```

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, three 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).
- Conditions of the type mixed (or "of exchange") who consist – in unsaturated – to impose a condition "external" for each principal unknown factor of hydraulics (p_c, p_g) as well as the coefficients of corresponding exchange. In fine, that consists in imposing a value on the "dual quantities" function of the external pressures and coefficients of exchange (in a linear way). The external pressures and the coefficients of exchanges are respectively indicated by the keywords PRE1_EXT and PRE2_EXT and COEF_11, COEF_12, COEF_21, COEF_22, by using the keyword factor ECHANGE_THM order AFFE_CHAR_MECA.
- 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,),
```

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```
                                          _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,
                   9460800000.0,12.6),);
```

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_VAPE LIQU_AD_GAZ
PRE1	p_{lq}	p_{lq}	$-p_{lq}$	p_g	$p_c = p_g - p_{lq}$
PRE2					p_g

Associated flows are:

For PRE1, FLUN_HYDR1 : $\left(M_w + M_{vp}\right).n = M_w^{ext} + M_{vp}^{ext}$

For PRE2, FLUN_HYDR2 : $\left(M_{ad} + M_{as}\right).n = M_{ad}^{ext} + M_{as}^{ext}$

For the conditions D'exchange, who exists only for modelings of the type unsaturated *HH2* , syntax will be then as on the following example:
```
ECH=AFFE_CHAR_MECA (MODELE=MODELE,
```

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```
ECHANGE_THM=_F (GROUP_MA=' DROIT',
                COEF_11= C11 , COEF_12= C12 , PRE1_EXT=1.E6,
                COEF_21= C21 , COEF_22= C22 ,  PRE2_EXT=1.E5, ),);
```
The loadings are then activated in STAT_NON_LINE via the keyword EXCIT in the following way:
```
              EXCIT= (_F (CHARGE= ECH, TYPE_CHARGE=' SUIV' ),),
```
Associated flows are then:

For PRE1, $\left(M_w + M_{vp}\right).n = C11\left(p_1 - p_1^{ext}\right) - C12\left(p_2 - p_2^{ext}\right)$

For PRE2: $\left(M_{ad} + M_{as}\right).n = C21\left(p_1 - p_1^{ext}\right) - C22\left(p_2 - p_2^{ext}\right)$

We go to 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 meshs) which one treats. For a more complete and more detailed outline in the way in which the boundary conditions are treated 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 AFFE_CHAR_MECA, the example below illustrates this kind of condition:

```
P_DDL=AFFE_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
$$x\,PRE1 + y\,PRE2 = z$$

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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

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

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

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

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, lenlinst):

    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=AFFE_MATERIAU (MAILLAGE=MAIL,
                        AFFE=_F (TOUT=' OUI',
                            MATER=MATERIAU,),
                        AFFE_VARC=_F (NOM_VARC=' DIVU',
                                EVOL=DEFVHY,),);

    else:

    MATEHY=AFFE_MATERIAU (MAILLAGE=MAIL,
                        AFFE=_F (TOUT=' OUI',
                            MATER=MATERIAU,),);
```

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```
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,),
                          COMPORTEMENT=_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,
                      AFFE=_F (TOUT=' OUI',
                           MATER=MATERIAU,),
                      AFFE_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,),
                             COMPORTEMENT=_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,),);
```

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```
        else:

            DEPLA=STAT_NON_LINE (reuse=DEPLA,
                                 MODELE=MODMEC,
                                 CHAM_MATER=MATEME,
                                 EXCIT=_F (CHARGE=CHARMEC,),
                                 ARCHIVAGE=_F (LIST_INST=UNPAS,),
                                 COMPORTEMENT=_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 H 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,

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	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'
    / 'GONF_ELAS'
    / '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 DEFI_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

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permeability relative and its derivative according to saturation. The user returns these curves via a series of formulas then called by `DEFI_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:

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

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

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` :

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

or by a cubic law for `HYDR_VGC`:

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

with in all the cases parameters n, Pr, Pe, Swr, $Smax$ defined in `DEFI_MATERIAU` :

n corresponds to the parameter `VG_N`
Pr corresponds to the parameter `VG_PR`
- Pe corresponds to the parameter `VG_P ENTR` (0 by default)
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, $C1$ in $Smax$, so as to avoid having to treat derivative of infinite values. Indeed, for $S = 1$:

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

and in the case of `HYDR_VGM`:

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

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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 $C1$ in this point.

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

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

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

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

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

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.

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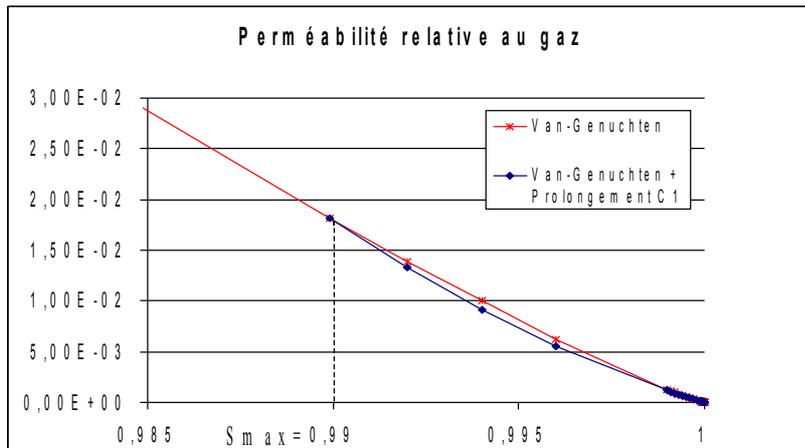
Figure 2.5.3-a: Example of prolongation of a relative permeability

For suction $S(Pc)$ and for $Pc < Pcmin$ (with $S(Pcmin) = Smax$) the curve is prolonged $S(Pc)$ by a hyperbole such as the curve is $C1$ in this point:
For $S > Smax$:

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

With A and B such that the curve is $C1$ in $Smax$.
There is thus well a decreasing curve which tends towards 1 when Pc tends towards $-\infty$. This treatment enables us to manage negative capillary pressures in Code_Aster (see the example Figure 2.5.3-b).
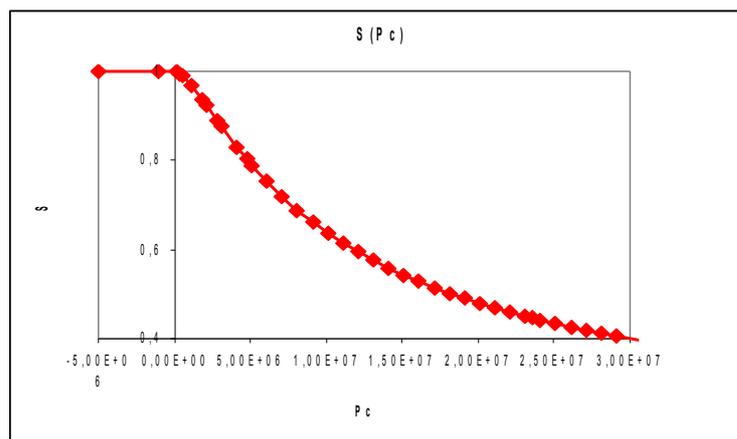
Figure 2.5.3-b: Example of prolongation for PC<0

$S(Pc)$ 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 chooses porous environments unsaturated, one cannot affect a 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', 'GONF_ELAS', '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', 'GONF_ELAS', '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:

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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,
            FICHIER=' 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,
            FICHIER=' 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

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

assignment of the model corresponding:

```
MODELQ4=AFFE_MODELE (MAILLAGE=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',),
              MAILLAGE=MAILQ4,),);
```

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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 one 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. The 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_MAILLAGE to define the patch
3) Possible modification of the type of meshs 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 maillor 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 meshs 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 "patchs 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 meshs 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, χ microscopic voluminal deformation and λ the multiplier of Lagrange:

Modeling	Type of meshs	Degrees of freedom	Position of the degree of freedom
D_PLAN_2DG	TRIA7, QUAD9	f_{ij}	At the tops of each element
		λ_{ij}	In the center of each element
D_PLAN_DIL	TRIA7, QUAD9	χ	At the tops of each element
		λ	In the center of each element
	TRIA6, QUAD8	χ	At the tops of each element
3D_DIL	TETRA10, HEXA20, PENTA15	χ , λ	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 as 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,),);
```

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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 solvor 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 ssll117.

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Annexe 1 Generalized constraints and internal variables

Constraints:

Number	Name of component Aster	Contents	Modelings
1	SIXX	σ'_{xx}	So mechanical (. M …)
2	SIYY	σ'_{yy}	So mechanical (. M …)
3	SIZZ	σ'_{zz}	So mechanical (. M …)
4	SIXY	σ'_{xy}	So mechanical (. M …)
5	SIXZ	σ'_{xz}	So mechanical (. M …)
6	SIYZ	σ'_{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…)

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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 (… THH2…)
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.

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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

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

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

The deduced variational formulation is given by

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

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

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

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

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

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

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

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

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

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, $\dfrac{p_{lq} - p_{lq}^0}{\rho_{lq}} = \dfrac{R}{M_{vp}^{ol}} T \ln\left(\dfrac{p_{vp}}{p_{vp}^{sat}(T)}\right)$, but this law is not used directly in Aster.

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The reference documents Aster do not say anything on what are the variables π_1 and π_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 $E_g^{*el} = \left(v, \varepsilon(v), \pi_1, \nabla \pi_1, \pi_2, \nabla \pi_2, \tau, \nabla \tau \right)$ is related to the vector of virtual displacement nodal $U^{*el} = \left(v, \pi_1, \pi_2, \tau \right)$ by the same operator Q_g^{el} that which connects between them the deformation $E_g^{el} = \left(u, \varepsilon(u), p_1, \nabla p_1, p_2, \nabla p_2, T, \nabla T \right)$ and nodal displacement $U^{el} = \left(u, p_1, p_2, T \right)$:
  - $E_g^{*el} = Q_g^{el} U^{*el}$
  - $E_g^{el} = Q_g^{el} U^{el}$

It is then clear that π_1 and π_2 are virtual variations of p_1 and p_2
From where the table:

$$p_1 = p_c \Rightarrow \pi_1 = \delta\, p_c = p_c^*$$
$$p_1 = p_{lq} \Rightarrow \pi_1 = \delta\, p_{lq} = p_{lq}^*$$
$$p_2 = p_{gz} \Rightarrow \pi_2 = \delta\, p_{gz} = p_{gz}^*$$

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.

$$p_c = p_{gz} - p_{lq} = p_c^{imp}$$
$$p_{gz} = p_{as} + p_{vp} = p_{gz}^{imp}$$

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 AFFE_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:

$$p_c = p_{gz} - p_{lq} = p_c^{imp}$$
$$p_1^{imp} = p_c^{imp}$$

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 π_2 unspecified and π_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

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the meaning of the distributions. One multiplies [éq A5.1- then1] by π_1 such as $\pi_1 = 0$ on $\partial\Omega_d$ one multiplies [éq A5.1-2] by π_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:

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

One from of deduced

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

- **Dirichlet** $PRE\,2$, **Neuman** $PRE\,1$

It is the case where one imposes a value on $PRE\,2$ and a value with flow associated with $PRE\,1$, 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 $M_{1_{ext}}$ this imposed quantity, which will be worth 0 if nothing is known as compared to $PRE\,2$. We will note $p_2 = p_2^{imp}$ the condition imposed on $PRE\,2$.

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:

$$\left(M_{lq} + M_{vp}\right).n = M_{1\,ext}\,\text{sur}\,\partial\,\Omega_d$$

With2.3 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:

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

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, μ such as:

$$-\int_\Omega \left(\dot{m}_{lq} + \dot{m}_{vp}\right)\pi_1\, d\,\Omega + \int_\Omega \left(M_{lq} + M_{vp}\right).\nabla\pi_1\, d\,\Omega - \int_\Omega \dot{m}_{as}\pi_2\, d\,\Omega + \int_\Omega M_{as}.\nabla\pi_2\, d\,\Omega +$$
$$+\int_{\partial\Omega_d} \mu^*\left(p_2 - p_1 - p_{lq}^{imp}\right) d\,\Gamma + \int_{\partial\Omega_d} \mu\left(\pi_2 - \pi_1 - p_{lq}^{imp}\right) d\,\Gamma \quad \forall\,\pi_1, \pi_2, \mu^*$$

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

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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 π_1 unspecified one multiplies [éq A5.1-2] by π_2 unspecified, one integrates by part, one carries the results found in [éq A5.3-2] and one obtains:

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

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:

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

From where one deduces:

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

A2.4 Case of boundary conditions mixed

We approach in this section the case of the boundary conditions mixed (or conditions of exchange) appliedS in the form of a condition of NeumanN. These conditions can relate to one or the other of the conservation equations or of course both.

The writing of flows is done then in the form:
$(M_{lq}+M_{vp}).n = M_{1ext} \text{ sur } \partial\Omega_d$ with $M_{1ext}=\lambda_{11}(p_1-p_1^{ext})-\lambda_{12}(p_2-p_2^{ext})$

and/or

$M_{as}.n = M_{2ext} \text{ sur } \partial\Omega_d$ with $M_{2ext}=\lambda_{21}(p_1-p_1^{ext})-\lambda_{22}(p_2-p_2^{ext})$

This condition is implemented in an explicit way (the value of *PRE1* and/or *PRE2* being taken at time precedent). These mixed conditions are thus applied like conditions of Neumann (cf previously).

With2.5 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:

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

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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:

$$-\int_\Omega \left(\dot{m}_{lq} + \dot{m}_{vp}\right)\pi_1 \, d\Omega + \int_\Omega \left(M_{lq} + M_{vp}\right).\nabla \pi_1 \, d\Omega - \int_\Omega \dot{m}_{as}\pi_2 \, d\Omega + \int_\Omega M_{as}.\nabla \pi_2 \, d\Omega +$$

$$+\int_{\partial\Omega_d} \mu^*\left(p_2 - p_{vp} - p_{as}^{imp}\right) d\Gamma + \int_{\partial\Omega_d} \mu\left(\frac{\partial p_{vp}}{\partial p_{lq}}\pi_1 + \left(1 - \frac{\partial p_{vp}}{\partial p_{lq}}\right)\pi_2\right) d\Gamma \quad \forall \pi_1, \pi_2, \mu^*$$

And one would find:

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

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

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