

## Realization of a calculation of prediction of rupture per cleavage

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### Summary

This documentation is intended to provide the necessary information to user wishing to simulate a rupture by cleavage while using *Code\_hasster*.

The definition of cleavage is initially pointed out. One presents then in turn the models present in *Code\_Aster* to predict this kind of rupture and of the methodological advices and setting in work. The models described here are in turn: Beremin, Bordet, Gp and Corre.

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## 1 Introduction

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Elastic breaking process, based on the classical criteria of rate of refund of energy, integral of contour  $J$  and of factor of intensity of the constraints  $K$ , does not allow, in the case general, to deal with the problems in which plasticity plays an important role. In this case, which remains field of research open in the great widths, other approaches must be installation. In the case of monotonous loading proportional, approaches with 2 parameters, as approaches  $(J, Q)$  or  $(K, T)$  ([1]) generally give satisfaction. Unfortunately, the field of validity of these approaches is limited to the loadings proportional.

This is why the elastoplastic breaking process, which must make it possible to extend the validity of the breaking process, is developed. The mechanism of cleavage (with confined plasticity) uses its attributions particularly.

This documentation aims to provide a methodological help to the use of the models of elastoplastic breaking process within the framework of the prediction of cleavage. It does not exempt to in no case reading of the reference documents and Use of Code\_hasster relating to the models and order of which it is question here.

The phenomenon of cleavage is initially quickly explained. Four models usable in Code\_hasster, two probabilists (Beremin and Bordet) and two determinists ( $G_p$  and Corre), are described in turn with assistances to their respective use. These models being of standard postprocessing of a thermomechanical calculation, it is appropriate that this calculation is most reliable possible, and thus that precautions, pointed out here, are taken.

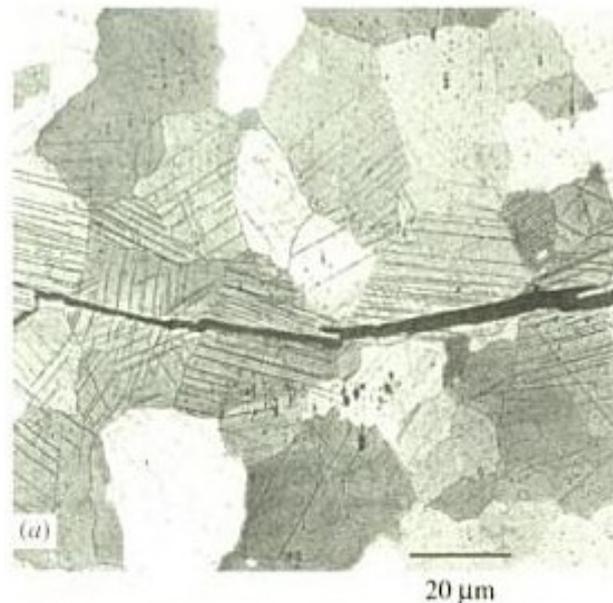
## 2 Short general information on cleavage

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This paragraph is in particular inspired by [2], to which one will be able to refer for more microstructural details in particular.

Cleavage is a mode of rupture whose principal mechanism is the separation of the atomic plans, practically without deformation. It is the principal mechanism of brittle fracture in metals, in particular in the case of low crystalline symmetries like the cubic ones centered or the hexagonal ones. This mode of rupture being competing with the plastic deformation, it is facilitated by a low temperature (the mechanisms of deformation then are activated). This led to the existence of a fragile transition (at low temperature) - ductile (at higher temperature). Among the models which are here defined, the two deterministic methods are currently tested in the case of the zone of transition in order to predict the risk of cleavage. This use requires however precautions; to our knowledge, no method can to date be regarded as reliable predicting the risk of cleavage in the zone of transition.

The morphology of the rough surfaces per cleavage corresponds to a transgranular propagation. It can be easily observed by microscopy, as on the Figure 2-1. It is frequently characterized by the presence of lines parallel with the direction of propagation, which one calls rivers.



**Figure 2-1: Microscopic facies of cleavage**

The rupture by cleavage, like the other modes of rupture per cracking, distinguishes in theory two mechanisms: starting and propagation. Starting corresponds to the development of one microscopic crack inside healthy metal; it generally allowed that this stage requires a rather weak preliminary plastic deformation, which generates a stacking of dislocations and a singularity of the constraints, and the attack of an ultimate stress of rupture, is noted henceforth  $\sigma_c$ . The propagation of the cracks of cleavage is unstable, high speed (about 40% speed of sound in metal), and must satisfy an energy criterion with type Griffith [3].

Cleavage not being accompanied by important deformations, it does not require a great energy, contrary to the ductile rupture. This is why the Charpy test, measuring impact strength (energy necessary to the breaking by shock of a standardized test-tube) makes it possible to distinguish these two types of rupture for the same material (see Figure 2-2). At low temperature, energy necessary to the rupture is weak: the mode of rupture is cleavage. At high temperature, energy necessary to the rupture is high: the rupture takes place by tear. The limiting temperature between these two phenomena is called temperature of transition; there are several definitions, which those based on a given energy level (one speaks for example about  $T_{k65}$ , which would be equal to approximately here  $-20^\circ C$ ).

The irradiation of metals induces an increase in the elastic limit and makes more difficult the stacking of dislocations, and *in fine* support cleavage: the temperature of transition from an irradiated material is higher than that of same material not irradiated. In the zone of transition, i.e. the beach of temperature close to this temperature of transition, the rupture can occur by cleavage, tear or a tear over a followed finite length by cleavage. The prediction of cleavage in zone of transition remains field of research: even if methodologies are proposed here, they still require validation and do not have to be seen like methods "turn-key".

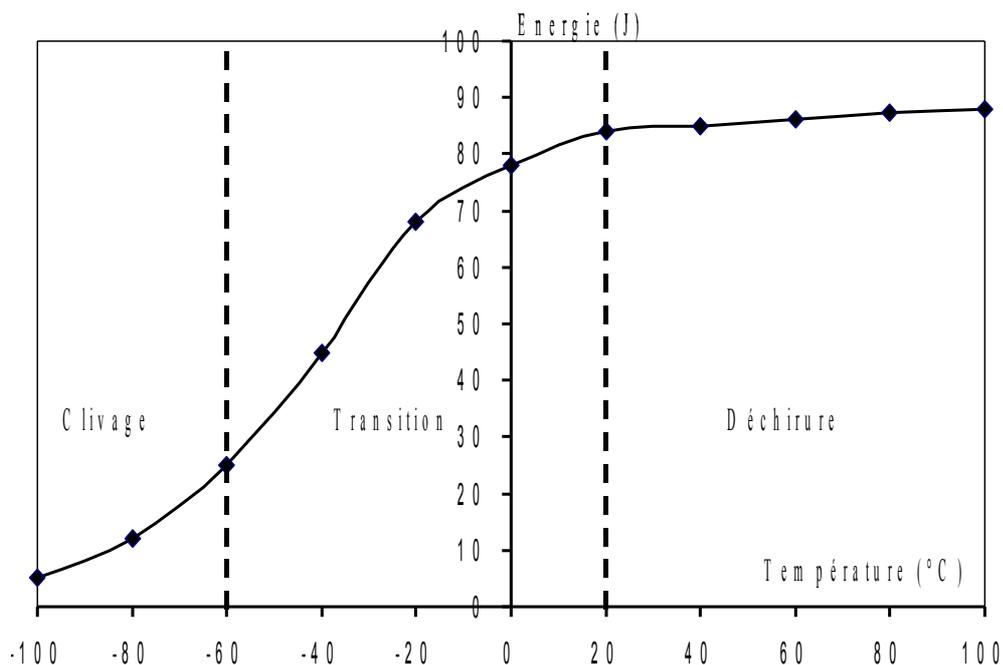


Figure 2-2: Curve of Fragile transition Ductile by Charpy test

### 3 Methodology of a calculation with the energy model Gp

The energy model  $G_p$  is developed at EDF R & D. It is deterministic and thus makes it possible to write a simple criterion of interpretation. It makes it possible to treat all the types of loading and takes into account of many effects (small defect, triaxiality, hot preloading), and of the studies to validate it ductile-brittle transition are in hand.

#### 3.1 Tally theoretical

The model énergétique  $G_p$  is initially based on the variational approach of the rupture suggested by Frankfurt and Marigo [4]. It makes it possible to define a criterion of starting validates in the field of cleavage whatever the type of loading. It is characterized by the representation of the crack by a notch, the principle of minimization of energy and applies that starting can be described by an energy criterion. It in particular makes it possible to take into account the effects small defects, of triaxiality and the effects of hot preloadings (which however are underestimated). For more details, one can refer to [5] or [R7.02.16]

One specifies here the essential components with the use of this approach in Code\_hasster, within the framework of the cleavage and the zone of transition.

#### 3.2 Grid necessary

In all the cases, the grid must comprise a defect (crack) represented by a notch (crack whose face is not a point but a half rings) initial ray  $R_0$ . This ray is a parameter to be identified. Its identification is described further. In the case of loading proportional, one can use a sufficiently small unspecified ray.

##### 3.2.1 In 2D

In 2D, the user has the choice between two types of grid.

In the first case, the grid must comprise specific zones of calculation called chips, each chip being defined by a group of meshes. An example of grid with chips is presented in Figure 3-1. The size of the chips must be provided by the user. One advises to use a depth of cut (size of mesh  $t_e$ ) to the maximum equalizes with the fifth of the initial ray of notch  $R_0$ .

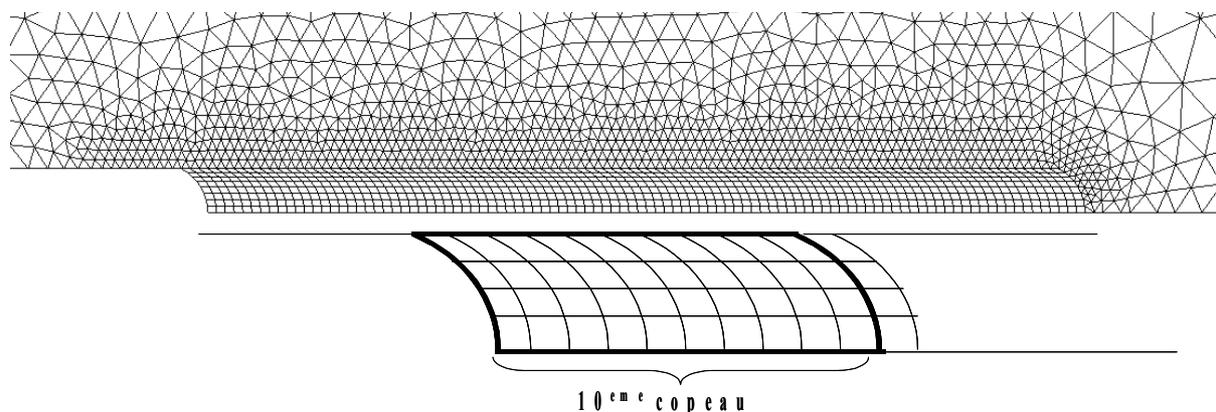
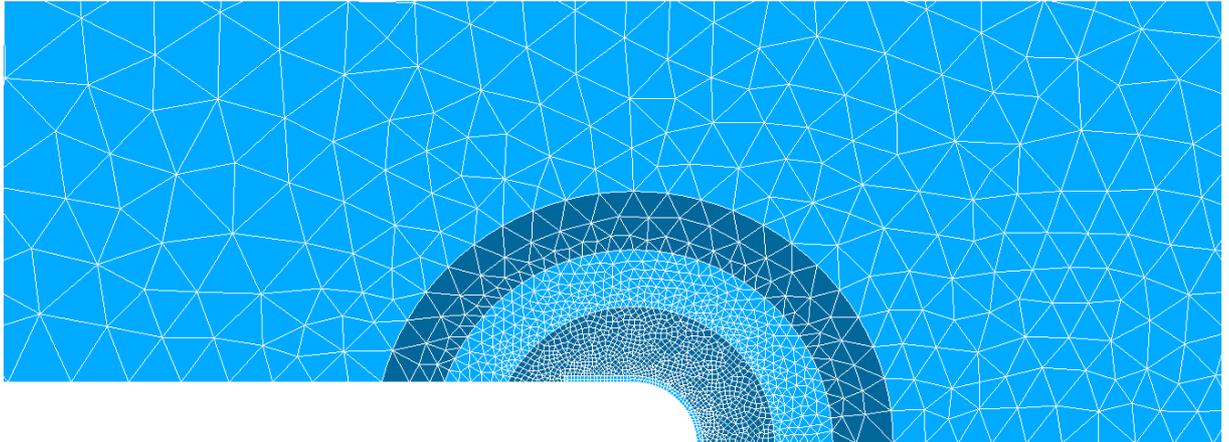


Figure 3-1 - Classical grid with definition of the chips.

The user can however use in 2D an unspecified grid (with representation of the defect by a notch) sufficiently refined in the zone close to the notch. The chips are then defined automatically with parameters users. An example of refined grid usable for the method is presented in Figure 3-2.



**Figure 3-2 - Free grid without definition of the chips.**

To finish, a user not having dedicated specific grid 2D can also use the order `RAFF_GP` to obtain a sufficiently fine and regular grid in the zone of interest of the notch (chips). The notch must be represented all the same geometrically, and the sufficiently regular grid in the zone of the chips, with “clean” meshes (slightly distorted).

### 3.2.2 In 3D

One of the principal difficulties of the use of this approach in 3D is due to the fact that it requires to have carried out a grid defining the zones of calculation known as chips and slice (see Figure 3-3). It is necessary that this zone is with a grid with hexahedrons. One advises to use a depth of cut (size of mesh  $t_e$ ) to the maximum equalizes with the fifth of the initial ray of notch  $R_0$  :

$$t_e \leq \frac{R_0}{5} \quad (1)$$

The concept of slice corresponds to an angular sector in the direction of propagation of the notch (see Figure 3-4).

In the case of a semi-elliptic face, it is advised to carry out a grid at least containing 16 slices on along the bottom of notch, even 32 or 64 if it is lengthened.

The grids are preferably quadratic, which allows, number of nodes given, a more precise calculation and to better collect the gradients of constraint.

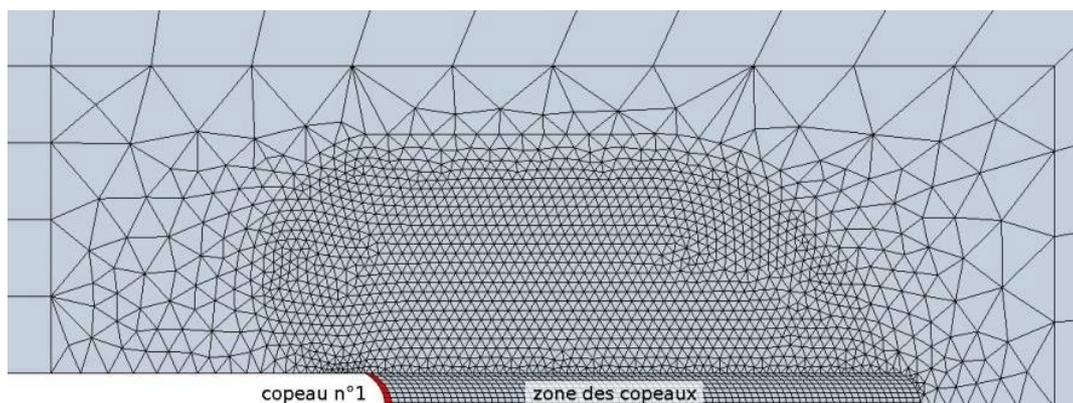


Figure 3-3: Definition of the chips: together of mesh of form equivalent to the face of notch.

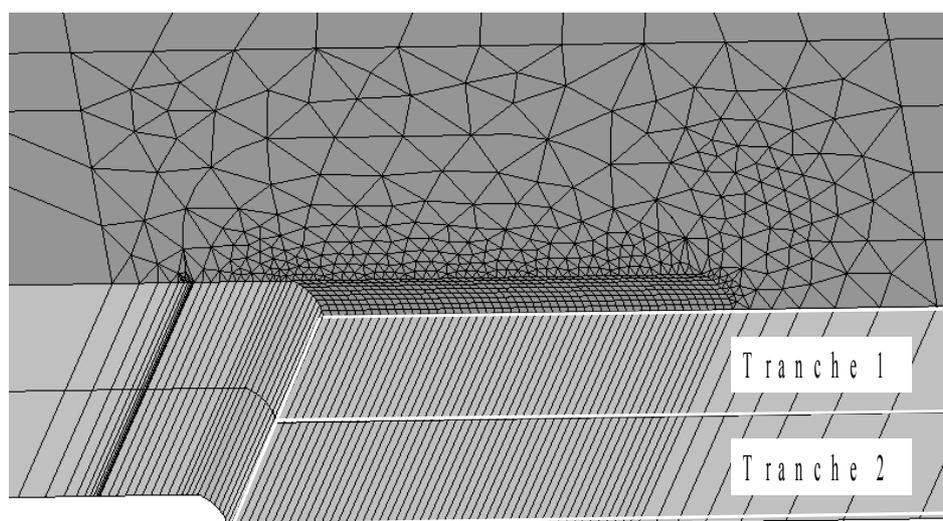


Figure 3-4: Definition of the zone of slice

As for the two-dimensional case with definition of the chips in the grid, the chips of the various slices must be defined by groups of mesh.

The groups of meshes chips must moreover be arranged in a list of groups of meshes arranged slice by slice in the following way (for  $p$  slices of  $N$  chips): tranche\_1\_copeau\_1, tranche\_1\_copeau\_2,..., tranche\_1\_copeau\_n, tranche\_2\_copeau\_1,..., tranche\_p\_copeau\_n.

### 3.3 Identification of the parameters

The energy model is based on two parameters: the initial ray of notch  $R_0$  and the critical parameter  $G_{pc}$ . These two parameters are to be identified starting from a test on test-tube CT.

One supposes known, for material considered:

- the Young modulus  $E$ ,
- the critical stress  $\sigma_c$ ,
- the energy of surface  $G_C$ .

The parameter  $G_{PC}$  is determined by simulation of a test on test-tube  $CT$  where the crack is represented by a notch of ray  $R$  given. This parameter corresponds to the space maximum value (on the whole of the chips of the whole of the slices) of the parameter  $G_P$  when the loading is such as  $G = G_C$ .

The approach of identification is the following one:

- grid with definition of the chips in 3D, or without definition of the chips in 2D
- realization of elastoplastic mechanical calculation; it is advised to use under-integrated elements (D\_PLAN\_SI, 3D\_SI...) to decrease the effects of incompressibility
- first post-treatment: calculation of the rate of refund of energy by the operator CALC\_G
- postprocessing of  $G_P$  via the order CALC\_GP

The syntax of the order CALC\_GP is the following one (one takes here the case 2D with grid comprising the groups of mesh of chips):

```
[table] = CALC_GP (
#Résultat mechanical calculation post-to treat and moments of postprocessing
    RESULT      =   resumeca,
    LIST_INST   =   moments,
#Table of shortened exit requested
    GPMAX      =   CO ('TABGPMAX')
#Définition of the zones of calculation (chips)
    TRANCHE_2D =_F (
        ZONE_MAIL = 'YES',
        GROUP_MA  = l_group,
        SIZE      = l_taille,
    )
)
```

One obtains at exit 2 tables: and tabgppmax.

Here is the detailed contents.

contains the values of  $G_P$  in any moment and place of calculation:

MOMENT	ZONE	ENER_ELAS	DELTAL	GP	MAX_INST
#Instant Indicator	Chip	Elastic energy	Distance to the bottom	Value of GP	
1.00000E+00	CO_1	0.004428	2nd-02	2.21402E-01	0
1.00000E+00	CO_2	0.009678	4th-02	2.41955E-01	1
3.00000E+00	CO_1	0.007208	2nd-02	3.60683E-01	0
3.00000E+00	CO_2	0.015359	4th-02	3.83966E-01	1

tabgppmax contains same following information, but only when MAX\_INST=1 :

MOMENT	ZONE	ENER_ELAS	DELTAL	GP	MAX_INST
#Instant Indicator	Chip	Elastic energy	Distance to the bottom	Value of GP	
1.00000E+00	CO_2	0.009678	4th-02	2.41955E-01	1
3.00000E+00	CO_2	0.015359	4th-02	3.83966E-01	1

If  $G = G_C$  at moment 3, one has then  $G_{PC}(R) = 0,38396$

Up to now, calculation was carried out for a value of ray of notch  $R$  data. However, the value obtained from  $G_{PC}$  depends on the selected ray of notch. In the absolute, it is thus necessary to renew the operation for various rays of notch, then to trace the dependence  $G_{PC}(R)$ . One adds the

line of slope then to it  $\frac{\sigma_c^2}{E}$  ; parameters to be chosen  $(G_{PC}, R_0)$  correspond to the point of intersection of the two curves (see Figure 3-5).

However, if the later study to carry out enters within the framework of a loading proportional monotonous, it is possible to arbitrarily choose the ray of notch of identification of  $G_{PC}$  (the ray must however be selected sufficiently small), and to carry out the study with this same ray and this same parameter  $G_{PC}$  ; in the past, many studies under loading proportional were carried out with an arbitrarily selected ray of notch enters 50 and 100  $\mu m$  .

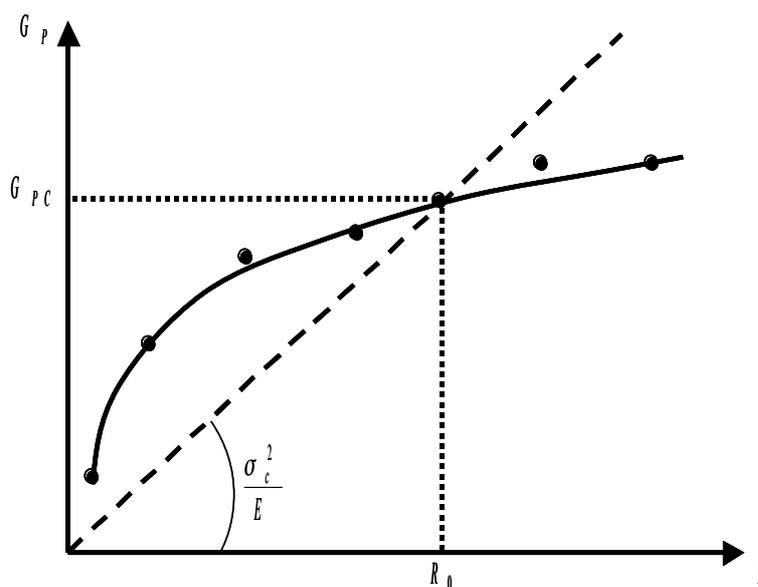


Figure 3-5: Curve of identification of the parameters of the energy model

The approach of identification presented here is valid for a given temperature. In any rigour, it would be necessary to identify the couple of the parameters  $(G_{PC}, R_0)$  for several temperatures in the range of interest of calculation. However, even if the temperature of the part evolves in the course of time, it is understood well that it is not possible to make evolve the ray of notch during calculation. This is why the total identification must be carried out on a temperature close to the temperature of future interest (that to which one wishes to carry out the prediction of cleavage); so of other temperatures are necessary, one will preserve the ray  $R_0$  initially identified and one will identify again only the breaking value  $G_{PC}$  .

### 3.4 Prediction of the cleavage of a structure

The energy model was validated for many situations in the zone of cleavage, but still requires tests of validation in the zone of transition (see Figure 2-2 for the definition of the zones of cleavage or transition).

The first question to be posed is the following one: will I carry out mechanical calculation (that to which I will apply my criterion of cleavage) in great or small deformations?

This choice will have to be deferred to the procedure of identification defined above: **the mechanical calculation of identification on CT will have to be carried out with the same type of deformations and the same ray as the study on structure.**

Methodology to be followed is the following one:

- to identify the parameters of the approach  $G_{PC}$  and  $R_0$  on CT (with notch of course).

- to carry out a grid of the structure of the type notches with chips, like defined in paragraph 3.2, with the ray of notch  $R_0$ .
- to carry out the mechanical simulation of the structure with the same type of deformation as that of identification, with preferably an under-integrated formulation (D\_PLAN\_SI, 3D\_SI...)
- post-to treat with the operator CALC\_GP.

Starting will take place when  $G_p$  reached, inside the zone of chips (it does not matter where), the value  $G_{PC}$ ; the breaking value is generally reached at a nonworthless distance from the face of crack.

## 4 Methodology of prediction of cleavage with the probabilistic model of Beremin

The model of Beremin has a high international recognition. It makes it possible to take into account of many effects (small defect, triaxiality, hot preloading) in complex situations of loading. Its principal "defect" is to be a probabilist, and thus more difficult of interpretation.

### 4.1 Tally theoretical

The model of Beremin is based on the existence of a mechanical constraint of cleavage. On the basis of this point, an estimate of the probability that a site of damage (microphone-defect) reaches the constraint of cleavage is established. By using an assumption of weak link (if a site breaks, the whole structure breaks), it is then possible to determine the probability of complete rupture of the structure starting from the plasticity and stress fields in her centre. For more details, one can refer to [R7.02.04] or [6].

One specifies here the essential components with the use of this approach in Code\_hasster, within the framework of the cleavage and the zone of transition.

### 4.2 Grid and modeling necessary

This model being based on the distribution of the constraints in a vicinity of the defect, it is theoretically necessary that preliminary mechanical calculation is most reliable possible. In practice, there exist two "schools" of use of the model. The school "historical", rather directed engineering, at the same time simpler and less expensive (see [7]) but less precise, and a more directed method research, more precise and reliable insofar as the mechanical fields are more precisely calculated, but at the cost much higher (see for example [8]). In both cases, the grids are preferably quadratic, which allows, number of nodes given, a more precise calculation and to better collect the gradients of constraint.

#### 4.2.1 Pragmatic modeling

In this modeling the defect is represented by a crack with a grid.

- To fix a size of mesh  $t_e$  about 50 with  $100\mu m$  in a zone where the model of Beremin is used. This choice makes it possible to have reasonable computing times as well as a good description of the mechanical fields.
- Réaliser a grid consequently, in the shape of grid around the defect (see Figure 4-1) with quadrangular elements (2D) or hexahedral (3D) of size  $t_e$  in the zone close to the bottom of defect;
- To fix the voluminal parameter of the law of Beremin, often noted  $V_0$ , about  $(50\mu m)^3$  with  $(100\mu m)^3$ . This parameter related on the microstructure and the distribution of the sizes of defect in material, must contain with minima a defect. The state of stress is regarded as homogeneous in this volume. There is no link enters  $V_0$  and cuts it of mesh if it is not that the latter gives one

characteristic distance on which the constraints will be homogeneous by calculation. In practice, in the implementation of the model, the choice of  $V_0$  do not impact the results.

- Utiliser if that is possible formalism large deformations (GDEF\_LOG) to avoid singular stress fields.

*Note: in great deformations logarithmic curves ( GDEF\_LOG ), the macro-order POST\_BEREMIN use the specific stress field  $T$ , while the macro-order POST\_ELEM use the stress field of Cauchy  $\sigma$  (see [R5.03.24]).*

- Utiliser an under-integrated quadratic formulation ( D\_PLAN\_SI, 3D\_SI... ) to minimize the effects related to the incompressibility (voluminal blocking in pressure in particular) with POST\_ELEM; it is from now on possible to carry out postprocessings of breaking process of cleavage with the elements incompressible (GRAD\_INCO) with POST\_BEREMIN [U4.81.31].

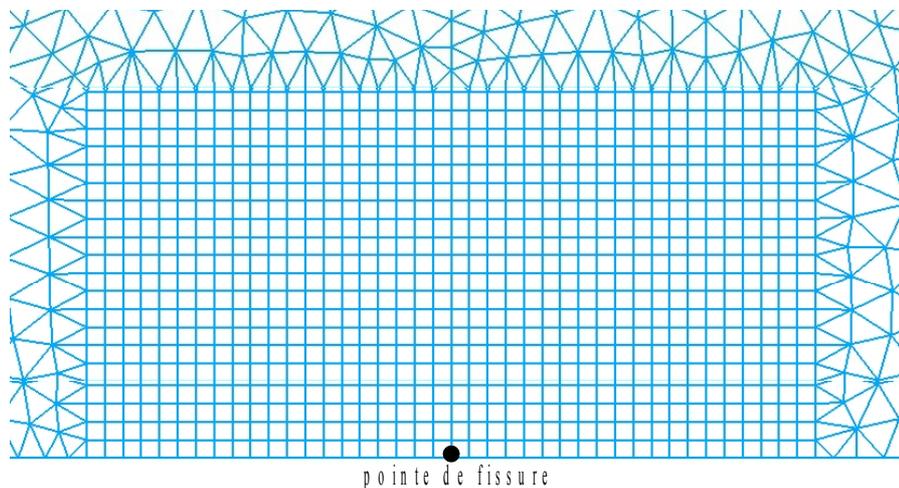


Figure 4-1: Classical grid 2D for the Beremin method

## 4.2.2 Modeling advanced for a reliable calculation of the fields in bottom of defect

This procedure is more difficult to set up. In order to obtain a rather precise calculation of the mechanical fields, the defect should not be represented by a crack (which generates a strong singularity), but by a notch of weak ray (not to disturb too much the solution compared to the crack).

The ray  $R_0$  must observe the condition known as of McMeeking [9].

With the final one, when that is possible, one proposes the following approach to carry out a mechanical calculation in a zone close to a defect:

- to identify the level of loading concerned and to evaluate it in term of factor of intensity of the constraints  $k_I$  ;
- to determine the ray of notch corresponding approximately to such a study by the formula  $R_0 = \frac{k_I^2}{10 E \sigma_Y}$ , with  $E$  Young modulus and  $\sigma_Y$  yield stress; the weaker the loading is, the more the ray owes the being!
- to carry out a grid consequently, of a form similar to that presented in Figure 4-2, with elements of size  $R_0/3$  or less in the zone close to the bottom to defect;
- to use a formalism great deformations (SIMO\_MIEHE for an isotropic work hardening (inalienable hasvec POST\_BEREMIN) or GDEF\_LOG in the other cases);

- to use under-integrated quadratic elements (with `POST_ELEM/WEIBULL` ) or elements incompressibleS `INCO` (with `POST_BEREMIN` ).

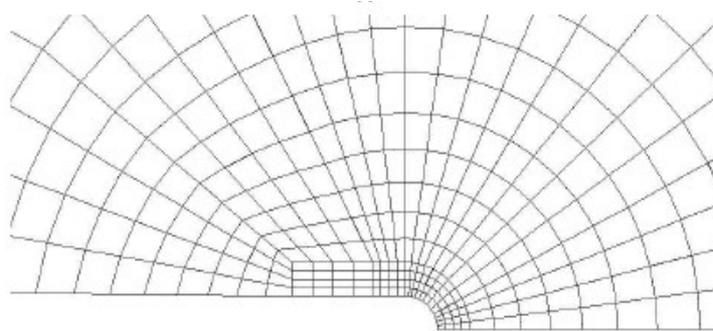


Figure 4-2: Grid for a precise mechanical calculation in bottom of defect

## 4.3 Identification of the parameters

Three material parameters enter the definition of the model of Beremin:  $V_0$ ,  $\sigma_u$  and  $m$ . In practice, the exhibitor  $m$  represented the dispersion of the defects likely to start brittle fracture and  $\sigma_u$  can be comparable to the constraint criticizes rupture of a ground volume  $V_0$ . Two parameters  $\sigma_u$  and  $m$  are characteristic of material considered. Ground volume  $V_0$  must be sufficiently large to include about ten grains and sufficiently small so that the stress field is quasi-homogeneous. One uses the same value of  $V_0$  in calculations `D_PLAN_SI`, `AXIS`, `3D_SI`, etc because the type of modeling (i.e. manner whose plasticized volume is calculated) is already defined by the operand `COEF_MULT` in `POST_ELEM` and in `POST_BEREMIN`.

identification of these parameters is not single, but depends on the choice made for modeling. Same manner, the parameters must be identified on a calculation showing the same characteristics as the calculation of prediction. One thinks here in particular of the option `CORR_PLAST`, which makes it possible to take into account refermeture of certain microscopic cracks when the deformations Shave important, and which must take the same value ('YES' or 'NOT') for the identification and the prediction.

The model being probabilist, the identification of the parameters requires in any rigour a battery of experimental tests very consequent. The more reliable the number of values of reference is important, will be the identification of the parameters. `Code_Aster` have a specific operator dedicated to the identification of the knowing model  $V_0$  : `RECA_WEIBULL`. An example of use of the order is available via the case test `ssna103`. The case test is carried out starting from a tensile test on a smooth cylindrical test-tube. The model can however also be identified on notched test-tube CT or axisymmetric. Mechanical calculation must be carried out so that the experimental moments of rupture are actually calculated and filed in the concept result.

Here here the ordering of the case test commented on:

```
T1=RECA_WEIBULL (
```

**#DEFINITION OF THE PARAMETERS TO BE READJUSTED; HERE,**

$\sigma_u, m$

```
LIST_PARA= ('SIGM_REFE', 'ME, ),
```

**#RESULTATS USE FOR THE IDENTIFICATION**

**#ICI, ONE IDENTIFIES WITH 3 TEMPERATURES, EACH RESULT BEING**

**#OBTENU AT THE TEMPERATURE IN QUESTION**

```
RESU= (
  _F (   EVOL_NOLI = U1,
        CHAM_MATER = CM50,
        TEMPLE = -50. ,

#LA EXPERIMENTAL RUPTURE WITH PLACE FOR
#LES LOADINGS AT THE MOMENTS DEFINED HERE
    LIST_INST_RUPT = (10. , 20. , 30. ,
                      40. , 50. , 60. , 70. , 80. , 90. , 100. ,
                      110. , 120. , 130. , 140. , 150. ,),
    MODEL = MO,
    ALL = 'YES',

#LE COEF_MULT TAKES INTO ACCOUNT SYMMETRIES AND
#L' THICKNESS OF THE SAMPLE
    COEF_MULT = 12.5664),
    .....),

#TYPE OF METHOD OF CALCULATING
    METHODE=' MAXI_VRAI ',

#DEFINITION OF THE MODEL USES,
#ICI WITHOUT PLASTIC CORRECTION
    CORR_PLAST=' NON',

#TYPE OF CONSTRAINT UTILISEE
#ON ADVISES ALWAYS TO USE SIGM_ELMOY
    OPTION=' SIGM_ELMOY',
    ITER_GLOB_MAXI=25,
    INCO_GLOB_RELA=1.E-3
)
```

## 4.4 Prediction of the cleavage of a structure

Once the identified parameters, calculation is carried out with the same recommendations as for the identification and with the same type of modeling (pragmatic or advanced).

2 operands are available (POST\_ELEM and POST\_BEREMIN) to calculate, at the wished moments and places, the constraint of Weibull and probability of rupture.

```
WEIB=POST_ELEM (

# DEFINITION OF THE TYPE OF CALCULUS PROBABILITY OF WEIBULL
WEIBULL=_F (CORR_PLAST=' NON',
            TOUT=' OUI',
            COEF_MULT=2.0,
            OPTION=' SIGM_ELGA',),

#DEFINITION OF THE RESULT, LOADING AND OF THE MOMENTS WITH
# TO CONSIDER
```

```
CHARGE=CHARG,
RESULTAT=U,
TOUT_ORDRE=' OUI ',);
```

One obtains a table as follows.

```
#-----
#ASTER 10.05.00 CONCEPT WEIB CALCULATE THE 7/1/2011 AT 16:34: 49 OF TYPE
#TABLE_SDASTER
```

NUME_ORDRE	INST	PLACE	ENTITY	SIGMA_WEIBULL	PROBA_WEIBULL	SIGMA_WEIBULL ** M
0	0.E+00	M	ALL	0	0	0
1	1.E+00	M	ALL	2,18E+003	1,48%	1,36E+080
2	2.E+00	M	ALL	2,18E+003	1,48%	1,36E+080
3	3.E+00	M	ALL	2,18E+003	1,48%	1,36E+080
4	4.E+00	M	ALL	2,90E+003	99,00%	1,30E+083

**Table 4.1: Table of exit of a post treatment of Beremin with POST\_ELEM**

```
BERE=POST_BEREMIN(
# DEFINITION OF THE TYPE OF CALCULUS PROBABILITY OF WEIBULL
COEF_MULT=2.0,
GROUP_MA = 'COUL_7',
DEFORMATION = 'GDEF_LOG',
FILTRE_SIGM= ' SIGM_ELGA',
#DEFINITION OF THE RESULT WITH TO CONSIDER
RESULTAT=ULOG,);
```

One obtains a table as follows.

```
#-----
#ASTER 15.03.25 CONCEPT 0000001b CALCULATE 9/21/2021 A 16:04: 34 OF TYPE
#TABLE_SDASTER
```

nume_ordre	inst	place	entity	sigma_weibu ll	proba_weibull	sigma_weibul ** m
1	1.E+00	COUL_7	GROUP_MA	2,18E+003	1,48%	1,36E+080
2	2.E+00	COUL_7	GROUP_MA	2,18E+003	1,48%	1,36E+080
3	3.E+00	COUL_7	GROUP_MA	2,18E+003	1,48%	1,36E+080
4	4.E+00	COUL_7	GROUP_MA	2,90E+003	99,00%	1,30E+083

**Table 4.2: Table of exit of a post treatment of Beremin with POST\_BEREMIN**

It is possible, for a level of loading given, to know the probability of rupture per cleavage of the structure.

It will be noted that in the procedures of determination of the risks of cleavage, one generally searches the loadings leading to probabilities of rupture of 5%,50% and 95%.

## 5 Methodology of prediction of cleavage with the probabilistic model of Bordet

The model of Bordet is relatively recent (2005). It was introduced in 2010 into *Code\_Aster*, thus this model does not have a very important experience feedback for the moment to EDF R & D. IL profited from the notoriety of the model of Beremin to penetrate the scientific world rather well, but remains confined in the industrial world. It is presented like better in the cases of loading with strong plastic deformations.

### 5.1 Tally theoretical

The model of Bordet is a modification of the model of Beremin, based on the same microstructural bases and the same assumption of weak link. The difference comes from the taking into account of plasticity. Dyears the model of Beremin, one supposes the creation of microscopic cracks at the time of the attack of the threshold of plasticity, and these microscopic cracks remain potentially active throughout the loading which is followed from there. However, in steels, the total rupture is mainly related to microscopic cracks lately created. It is thus advisable to take into account the level of plastic deformation reaches at every moment. In the model of Bordet, this is taken into account by considering that the probability of rupture by cleavage is the product of the probability of nucleation and propagation at the same moment. For more details, one will be able to refer to [R7.02.06] and [10].

### 5.2 Grid and modeling necessary

This model being a modification of the model of Beremin, the same recommendations can be made. One will thus refer to the Paragraph 4.2 .

### 5.3 Identification of the parameters

The model of Bordet has for principal defect its significant number of parameters material to identify: 7 in its full version, and 6 in its version simplified (accessible by `PROBA_NUCL = 'NOT'` ).

The first three parameters,  $V_0$ ,  $\sigma_u$  and  $m$  have the same meaning as in the model of Beremin; however, the author specifies that their respective value is not inevitably that of the classical model of Beremin...

With those is added a constraint threshold of cleavage  $\sigma_{th}$  , which can be taken equal to the critical stress of rupture  $\sigma_c$  useful for the identification of the energy model, and the yield stress  $\sigma_{ys}$  material with a temperature of reference and like a function of the temperature and speed of plastic deformation.

The last parameter, useful that in the case of the complete model, is the plastic deformation of reference of cleavage,  $\varepsilon_{p,0}$  , for which a microscopic crack of cleavage, nucleate by plastic deformation, is disabled if it immediately did not generate the rupture. In practice, the authors of the model themselves free themselves from this parameter... We thus advise, unless obtaining a value, to use the version of the model from it who does not require this parameter.

With final, a possibility is to use the version without probability of nucleation (`PROBA_NUCL = 'NOT'` ), to use the parameters  $V_0$ ,  $\sigma_u$  and  $m$  of Beremin (procedure described in Paragraph 4.3 ), the breaking stress and yield stresses identified on simple tensile test at various loading rates.

The other possibility, more delicate, is to simulate at the same time tests on CT and Charpy test-tube and to identify the whole of the parameters starting from the experimental data.

In both cases, one will be able to use a pragmatic or advanced modeling (see Paragraph 4.2), which leads to different values.

## 5.4 Prediction of the cleavage of a structure

As for the model of Beremin, the prediction of cleavage must be made while following the same approach as the identification (pragmatic or advanced).

The operand then is used `POST_BORDET` to calculate, at the wished moments and places, the constraint of Weibull and probability of rupture. One can refer again to the case test `ssna108a` for an example. The order `POST_BORDET` employee is commented on below.

```
BORDET=POST_BORDET (
    #DEFINITION OF the RESULT, the PLACE (here all the structure), MOMENT
WITH
    #UNE ABSOLUTE PRECISION OF 0.0001
    RESULTAT=U,
    TOUT=' OUI ',
    INST=9.9999,
    CRITERE=' ABSOLU ',
    PRECISION=0.0001,
    #UTILISATION OF THE MODEL SIMPLIFIES
    PROBA_NUCL=' NON ',
    #PARAMETRES MATERIALS
    PARAM=_F (M=8.,
        SIG_CRIT=600,
        SEUIL_REFE=555.,
        VOLU_REFE=1.E-3,
        SIGM_REFE=SIGU,
        SEUIL_CALC=SIGY,
    ),
    # UNIFORM TEMPERATURE CONSIDEREE IN THE PART
    TEMP=20,
)
```

The following table result is obtained:

```
#
#-----
#
#
#ASTER 10.05.00 CONCEPT BORDET CALCULATE THE 7/4/2011 AT 11:41: 55 OF TYPE
#TABLE_SDASTER
INST          SIG_BORDET          PROBA_BORDET
#INSTANT      CONSTRAINT OF BORDET          PROBABILITY OF CLEAVAGE
1.00000E+00   0.00000E+00                   0.00000E+00
2.00000E+00   0.00000E+00                   0.00000E+00
3.00000E+00   0.00000E+00                   0.00000E+00
4.00000E+00   7.21802E+02                   3.21879E-05
5.00000E+00   1.03164E+03                   5.60360E-04
6.00000E+00   1.30243E+03                   3.61088E-03
7.00000E+00   1.54241E+03                   1.38970E-02
8.00000E+00   1.73051E+03                   3.45253E-02
9.00000E+00   1.88667E+03                   6.77310E-02
1.00000E+01   2.02247E+03                   1.15112E-01
-            0.00000E+00                   0.00000E+00
```

It is then possible to trace the probability of rupture of the model of Bordet according to the loading. For the model of Beremin, the probabilities of 5%,50% and 95% are generally considered.

## 6 Methodology of prediction of cleavage with the model of Corre

The model of Corre is a model developed by Commissariat à l'Energie Atomique (ECA) with a principal aim qualitatively to characterize the starting (or the propagation) of a defect: cleavage or ductile. It is currently in the course of validation by the ECA, is always prone to modifications/enrichments and is used mainly in zone of ductile-brittle transition. It is not for the moment not the object of an order dedicated in *Code\_Aster*, but can however be used by "diverted" means clarified here. These diverted means will be made very soon simpler by programmed evolutions of code.

### 6.1 Tally theoretical

The model of Corre is based on arguments close to those of Beremin and enters within the framework of the approaches known as "local". It is based on the distribution of the constraints around the defect to determine if starting will be stable or unstable (cleavage). He does not have on the other hand authority to determine the moment of starting, but well his type. To define the moment of starting, it is generally coupled with a classical method based on the integral  $J$  in particular. For more details, one will be able to refer to [11].

### 6.2 Grid and modeling necessary

This model being based on the distribution of the constraints in a zone close to the bottom of defect (notch or crack), it is necessary to take a care particular to mechanical calculation. Moreover, the decisive criterion the moment of starting being based on the rate of refund of energy, it is appropriate to respect the advices with the good progress of a calculation of this type, given in [U2.05.01]. The ECA uses quadratic grids of type fissures free, with sizes of mesh around the defect of 50 with  $100 \mu m$ . In order to increase the quality of the result, in particular for the calculation of the parameters of breaking process by the method  $\theta$ , one advises however to use is a grid such as defined in Paragraph 4.2.2, that is to say a grid of the type fissures refined in bottom of defect, and preferably radiant for a better calculation of the rate of refund of energy  $G$ .

### 6.3 Identification of the parameters

The model of Corre is based on two parameters material: an ultimate stress noted here  $\sigma_{LC}$  and a limiting volume noted here  $V_{th}$ . The first parameter is identified starting from the experimental data of rupture of a Notched Axisymmetric test-tube whereas the second is identified on the simulation of a test-tube CT.

By assumption, the ultimate stress  $\sigma_{LC}$  is supposed to be independent of the temperature. In order to determine it, it is advisable to have tensile tests on test-tube AE for a sufficiently low temperature so that it breaks in cleavage (in practice, the temperature is generally about  $-150^\circ C$ ).

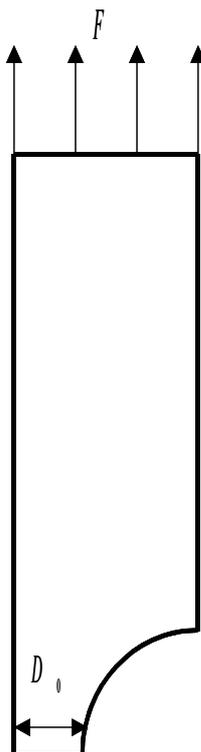
One as follows defines the average constraint in rupture:

$$\sigma_{moy} = \frac{4F}{\pi D_0^2 \left(1 - \frac{\Delta D}{D_0}\right)}$$

With the notations of the Figure 6-1.

One then determines the smallest average constraint at the instant of the failure of the various tests, and one defines:

$$\sigma_{LC} = 1.2 \text{Min}(\sigma_{moy})$$



**Figure 6-1: Tensile specimen for identification of the model of Corre**

Identification of the second parameter,  $V_{th}$ , the knowledge of test results of tensile requires on test-tube CT at low temperature (is needed that the rupture takes place for a very weak propagation of the crack), i.e. has *minimum* the value of the rate of refund of energy to rupture.

Two digital simulations 2D of the test are carried out. A first in small deformations (for the calculation of the rate of refund of energy), and a second in great deformations (for the calculation of  $V_{th}$ ). The curve then is plotted  $J$ /ouverture of defect for simulation in small deformations. One places oneself at the value of  $J$  with the rupture and one determines the opening of the defect  $ouv_{rup}$  on this level of loading.

On simulation in great deformations, one seeks the level of loading such as the opening is equal to  $ouv_{rup}$ . For this level of loading, one determines the volume of matter on which the constraint exceeds the value  $\sigma_{LC}$ . This stage can be realized via the order POST\_ELEM in the following way:

```
VOLUM=POST_ELEM (
    #DEFINITION OF THE MODEL AND THE RESULT
    MODELE=MOD,
    RESULTAT=EVOL,
    #DEFINITION OF THE MOMENT CONSIDERS
    INST= 1,
    #C' IS THE KEYWORD VOLUMOGRAMME WHICH SHOULD BE
    EMPLOYED
    VOLUMOGRAMME= (
        #ON POST-TRAITE ON THE WHOLE STRUCTURE
        _F (TOUT=' OUI',
        #ON LOOKS AT THE PRINCIPAL CONSTRAINT MAX
        NOM_CHAM=' SIEQ_ELGA',
        NOM_CMP = ' PRIN_3',
```

**#ON ADVISES TO TAKE MANY INTERVALS**

```
NB_INTERV=50, ),
), )
```

One obtains at exit a table containing many information at the place and the time of the post treatment; one concentrates here on the columns which interest us:

RESULT	NOM_CHAM	...	NOM_CMP	...	BORNE_INF	BORNE_SUP	DISTRIBUTION
					LIMIT INF OF THE INTERVAL	LIMIT SUP OF THE INTERVAL	RELATIVE VOLUME OF THE INTERVAL
EVOL	SIEQ_ELGA	...	PRIN_3	...	-1.51895E+02	-1.50910E+02	2.98596E-10
EVOL	SIEQ_ELGA	...	PRIN_3	...	-1.50910E+02	-1.49925E+02	0.00000E+00
EVOL	SIEQ_ELGA	...	PRIN_3	...	-1.49925E+02	-1.48940E+02	0.00000E+00
...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...
EVOL	SIEQ_ELGA	...	PRIN_3	...	8.30432E+02	8.31417E+02	4.21426E-09
EVOL	SIEQ_ELGA	...	PRIN_3	...	8.31417E+02	8.32402E+02	1.41899E-09
EVOL	SIEQ_ELGA	...	PRIN_3	...	8.32402E+02	8.33388E+02	3.88076E-09

**Table 6.1: Table of exit for the model of Corre**

One summons then the distribution for the values of constraints higher than  $\sigma_{LC}$ . For example here if  $\sigma_{LC}=830\text{MPa}$ , one summons the three last distribution, that is to say  $9.51401\text{E}-09$ . One multiplies this figure by the total volume of the part, and one obtains the parameter  $V_{th}$ .

The identification of the parameters is summarized as follows:

- on tensile tests on AE at low temperature, to determine the average constraint with rupture  $\sigma_{moy}$ ;
- in deducing the parameter  $\sigma_{LC}=1.2 \text{Min}(\sigma_{moy})$ ;
- to carry out a simulation, in 2D small deformations, of traction on test-tube CT which one knows it  $J$  with rupture;
- to determine the opening of defect when it  $J$  with rupture is reached ( $J$  calculated by CALC\_G);
- to carry out a simulation, in 2D great deformations, same test on CT;
- to determine the level of loading for which the opening of the defect equalizes the opening to rupture obtained in small deformations;
- on this level of loading, to use the order POST\_ELEM to know the volume of matter on which the maximum principal constraint exceeds the constraint  $\sigma_{LC}$ : this volume is equal to  $V_{th}$  (attention with symmetries: a multiplicative factor must be added to give an account of symmetries).

## 6.4 Prediction of the cleavage of a structure

As for the other models, it is necessary to use the same type of simulation as that carried out for the identification of the parameters (crack or fine notch).

One then carries out two thermomechanical calculations of the structure: one in small deformations, the other in great deformations.

Calculation in small deformations makes it possible to know the loading of starting, which is such as the integral  $J$  it reaches  $J$  with rupture (in general, the ECA uses the parameter  $J_{0.2}$ , corresponding to the value of  $J$  for a starting of 0.2mm on CT). This level of loading, one determines the opening of the defect.

Calculation in great deformations makes it possible to know the nature of starting; one places oneself on a level of loading such as the opening in great deformations is equal to the opening in small

deformations when it  $J$  with rupture is reached. This level of loading, one determines the volume of

matter  $V_{LC}$  on which the maximum principal constraint exceeds  $\sigma_{LC}$  : 
$$V_{LC} = \frac{\sum_i (V_i \vee \sigma_i \geq \sigma_{LC})}{V_{total}}$$

However, the parameter  $V_{th}$  was identified on tests 2D. Moreover, one suspects that if the face of crack has an infinite length, volume  $V_{LC}$  of going beyond will also tend towards the infinite one. This

is why volume  $V_{LC}$  must be divided by the length of the face of crack  $L_{front}$ . If  $\frac{V_{LC}}{L_{front}} < V_{th}$ , then

cleavage cannot take place, and starting will be ductile; if on the contrary  $\frac{V_{LC}}{L_{front}} > V_{th}$ , then the risk

of cleavage is nonnull and increases with  $V_{LC}$ . There exists an expression of the probability of cleavage according to  $V_{LC}$ , but this one was not sufficiently validated until now so that we make mention of it here. It however is described in [11].

## 6.5 Precautions and limits of this approach

From our point of view, this approach presents some limits and precautions which are quickly evoked here.

First of all, the limiting loading of starting is defined by the integral  $J$ ; this one being calculable rigorously only in elasticity (linear or not), the loading of starting cannot theoretically be given when one leaves elasticity. However, in the case of loading proportional monotonous, elastoplastic calculation can be regarded as nonlinear rubber band, and the calculation of  $J$  is valid. At all events, the method does not make it possible to predict the moment of starting for an unspecified loading.

Moreover, it is appropriate, to use the model completely, to carry out a calculation in small deformations and a calculation in great deformations, and to establish a link starting from the openings of defect in both cases. This kind of analogy, although current, is not entirely satisfactory.

These the first two remarks could be circumvented by using another criterion of determination of the calculable loading of starting in great deformations and valid for an unspecified loading. Unfortunately, it is not for the moment not possible.

On the level of the type of starting itself, the criterion is based on a volume of going beyond a breaking value of constraint in the zone close to the defect. However, in the zones close to the defect, and even more when this one is modelled by a crack, the calculation of the constraints is difficult because of the generated singularities and the problems of incompressibility. It is thus advisable to visualize the constraints (in particular hydrostatic, not equivalent) at the bottom of defect and to make sure that their distribution is physical. A common practice is to carry out the average of the constraints by element and to make use of it for calculation of volume; it will be pointed out that the average of two false results is not necessarily right.

## 7 Conclusion

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In Code\_aster, the prediction of cleavage can be realized with four models; three of them (Beremin, Bordet, Corre) are based on a criterion in constraint (approach known as local), the last ( $G_p$ ) being based on elastic energy (approach known as energy). Their respective fields of validity make it possible to sweep the complex situations of loading, in particular the cases of loading nonproportional. Calculations in zone of ductile/fragile transition raise more difficulty, and still deserve rather broad validation.

The principal council is to take care that thermomechanical calculation proceeds the best possible one. If the mechanical fields are calculated in a too approximate way, the quality of the predictions will be seen some affected.

The second council is to confront the predictions of several of the approaches, and, as for all the digital simulations, to carry a critical glance on the got results.

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