

# **FINITE ELEMENT MODELLING OF A SMOOTH TENSILE SPECIMEN AND A COMPACT TENSION SPECIMEN WITH THE GURSON-TVEERGARD-NEEDLEMAN AND ROUSSELIER MICRO-MECHANICAL MODELS**

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## **ABSTRACT**

This paper summarises CEA’s DMT contribution to the Phase II Round Robin organised by GKSS within the ESIS TC8 Committee on Numerical methods. The overall objective of this Round Robin is to investigate the ability of micro-mechanical models to predict ductile tearing in compact tension specimens made of the German designation ferritic 22 NiMoCr 3 7 steel. The purpose of Task A1 is to identify critical micro-mechanical damage parameters from FE analyses of a standard smooth tensile specimen. These parameters are then used in Task A2 to predict the  $J_R$  curve for a 20% side grooved CT25 specimen. The simulated results are then compared with available experimental data in order to draw conclusions and recommendations. Both the Rousselier and the Gurson-Tveergard-Needleman models, available in CEA’s finite element code CASTEM 2000, have been used.

## **KEYWORDS**

Elastic-plastic Fracture Mechanics, Ductile Tearing, Finite Element Micro-mechanical Modelling, Local Approach

## **INTRODUCTION**

The work reported in this paper is concerned with CEA’s DMT (Department of Mechanics and Technology) contribution to the Phase II Round Robin organised by GKSS within the ESIS TC8 Committee on Numerical methods. The overall objective of this Round Robin is to investigate the ability of micro-mechanical models to predict ductile tearing in compact tension specimens made of the German designation ferritic 22 NiMoCr 3 7 steel. This Round Robin follows a 1<sup>st</sup> phase, started in 1994 and accomplished in 1995. The results can be found in [1]. The objective of that Round Robin was to study the ability of micro-mechanical models and local approach to describe fracture phenomena including ductile tearing and cleavage for round tensile specimens only. In 1996, CEA and MPA Stuttgart in Germany performed the Phase I calculations [2] using the Rousselier model [3] and the FE code CASTEM 2000 [4].

The second phase of this Round Robin has started in August 1997. It consists in investigating the ability of micro-mechanical models to predict ductile tearing and cleavage in CT (compact tension) specimens, made of the same material than studied in phase 1. Phase 2 is subdivided in four tasks as follows :

1. Task A1 : Numerical analysis of a standard smooth tensile specimen to characterise the material and identify critical damage parameters for ductile tearing at 0°C.
2. Task A2 : Numerical simulation of ductile crack growth in a CT specimen using the critical damage parameters identified in task A1.
3. Task B1 : Numerical analysis of a notched tensile specimen to characterise and identify critical damage parameters for cleavage at low temperature.
4. Task B2 : Numerical simulation of a CT specimen using the critical damage parameters identified in task B1.

This paper describes the results obtained for Tasks A1 and A2 only.

## CONSTITUTIVE EQUATIONS

The constitutive equations of the two models used for the Round Robin are presented in the following. They include the Rousselier model and the GTN (Gurson-Tveergard-Needleman ) model [5, 6], both available in CASTEM 2000.

### *Rousselier Model*

The constitutive equations of the Rousselier model are based on the Von Mises yield condition extended for porous media :

$$f(\sigma, R, f) = \frac{\sigma_{eq}}{1-f} + D \cdot \sigma_1 \cdot f \cdot \exp\left(\frac{\sigma_h}{(1-f)\sigma_1}\right) - R(p)$$

$$1-f_0$$

$f_0$  is the initial void volume fraction,  $f$  is the void volume fraction,  $R(p)$  is the tensile curve of the material and  $p$  the cumulated plastic strain,  $\sigma_{eq}$  is the Von Mises equivalent stress,  $\sigma_h$  is the hydrostatic stress,  $D$  is an integration constant for the model and  $\sigma_1$  is a stress characterising the resistance of the material matrix. The evolution of the void volume fraction depends on the plastic strain rate and is defined by  $\dot{f} = (1-f) \cdot \text{tr} \mathcal{E}^p$  where  $\mathcal{E}^p$  is the plastic strain rate tensor. In this model, no account is given to nucleation and an initial void volume fraction  $f_0$  has to be specified. The Rousselier model, as implemented in the code, includes a modification proposed by Seidenfuss [7] to account for the coalescence of voids. This modification allows to perform fracture mechanics calculations [8] and consists in the following :

- if  $f = f_0$  damage free material,
- if  $f_0 < f < f_c$  damaged material where  $f_c$  is the critical void volume fraction,
- if  $f = f_c$  fully damaged material, coalescence. The stresses at the Gauss points are forced to 0.

### *GTN Model*

The constitutive equations of the GTN model are also based on the Von Mises yield condition extended for porous media :

$$f(\sigma, R, f) = \sigma_{eq}^2 - R(p)^2 \left[ 1 + (q \cdot f_*)^2 - 2 \cdot q \cdot f_* \cdot \cosh\left(\frac{3 \cdot \sigma_h}{2 \cdot R(p)}\right) \right]$$

$f_*$  is the damage function defined by  $f_* = \mathcal{E}_{nucleation}^* + \mathcal{E}_{growth}^*$  where  $\mathcal{E}_{nucleation}^*$  is the nucleation contribution to the void volume growth rate and  $\mathcal{E}_{growth}^*$  is the growth contribution to the void volume growth rate. The growth contribution to the void volume growth rate is defined by  $\mathcal{E}_{growth}^* = (1-f) \cdot \text{tr} \mathcal{E}^p$  where  $\mathcal{E}^p$  is the plastic strain rate tensor and  $f$  is the void volume fraction. If nucleation is neglected, the damage function in the GTN model is defined by :

$$f_* = \begin{cases} \text{for } f \leq f_c & f \\ \text{for } f > f_c & f_c + K(f - f_c) \end{cases} \quad \text{with } K = \frac{f_u - f_c}{f_f - f_c}$$

$f_c$  is the critical void volume fraction at which coalescence occurs,  $f_u$  is the ultimate void volume fraction at which the material loses its load bearing capacity with  $f_u = 1/q$  and  $f_f$  is the void volume fraction at final fracture. In this model, nucleation may occur as a decohesion process between the metal matrix and the inclusions present in the matrix material. It can be controlled either by accumulated plastic strain or by the hydrostatic stress. The nucleation contribution to the void volume growth rate is expressed by  $\dot{\epsilon}_{\text{nucleation}} = B \cdot (K(p) + \bar{\epsilon}_n) + D \cdot \dot{\epsilon}_{\text{eq,mat}}^p$ . In this equation, the B coefficient controls nucleation by the hydrostatic stress and the D coefficient controls nucleation by the accumulated plastic strain in the material matrix  $\dot{\epsilon}_{\text{eq,mat}}^p$ . The expressions for B and D can be found in [5, 6].

## MODEL PARAMETERS IDENTIFICATION PROCEDURE

The procedure developed and adopted by CEA to identify micro-mechanical damage parameters for ductile crack extension in ferritic or austenitic steels is outlined in Figure 1. It is expected that the results obtained with that Round Robin will be used to draft an ESIS recommendation which will include coupled damaged models and their application to cracked bodies. It will be an extension of the ESIS P6-98 guideline [9] for which the application is restricted to crack free specimens and components.

With the exception of the material stress-strain curve which has to be first determined from tensile tests on smooth tensile specimens, the parameters to identify, regardless about the constitutive equations of the model used for the analysis, are the initial void volume fraction  $f_0$  and the element size  $L_c$  to be used for the material at the crack tip and along the crack growth path. The initial void volume fraction can be determined either from metallographic analysis of the material microstructure or from a chemical analysis of the material together with the Franklin formulae [10]. A FE (finite element) analysis can then be undertaken in order to finely tune the  $f_0$  value. It is done in such a way that the simulations allow to reproduce exactly the experimental rupture points observable on the load versus diametrical contraction curve measured with notched tensile specimens with different stress triaxiality ratios. For  $f_c$ , the critical void volume fraction, a value included between 0.05 and 0.1 is recommended for ferritic and austenitic steels.

The average distance between inclusions is modelled in the FE analysis with calibrated square elements which are used along the crack growth path. A first estimation of  $L_c$  can be obtained from a metallographic analysis of the material microstructure (estimation of the number of inclusion per unit of volume  $N_v$ ) and  $L_c = 2/\sqrt[3]{N_v}$  for 8 nodes reduced integration elements. A FE analysis can then be undertaken in order to finely tune the value of  $L_c$ . It is done in such a way that the simulations allow to reproduce exactly both the load versus  $V_{LL}$  (load line displacement) curve and the material  $J_R$  curve. In the calculation, J has to be determined by the computation of a far-field J-integral. A typical value for  $L_c$  is included between 0.1 and 0.5 for ferritic and austenitic steels.

For these calculations, a formulation based upon the Mises Prandtl Reuss constitutive equations with the normal flow rule applied to the yielding surface, a large displacement theory consisting in updating the stiffness matrix at each increment and a large strain analysis (Truesdell or Jauman derivation formulation) are recommended.

## NUMERICAL SIMULATION OF A SMOOTH TENSILE SPECIMEN

The mesh used for the computation follows the Round Robin specifications : only an axisymmetric quarter section of the smooth tensile specimen is modelled with 260 isoparametric quadratic axisymmetric 8 nodes elements with 4 Gauss points and 853 nodes. In the necking section, 10 elements are used together with a small radial imperfection corresponding to  $\Delta D = 0.005 D_0$  to insure strain localisation and necking at half

length of the specimen. This imperfection is distributed over 8 elements in the axial direction. The loading is simulated as an homogeneous axial prescribed displacement of the upper edge of the mesh.

A number of simulations were performed with the Rousselier model as the initial void volume fraction specified in the Round Robin ( $f_0=2E-3$ ) was found to be much too large when comparing the predictions with the experimental data. For the Rousselier model,  $D=2$ ,  $\sigma_1=445$  MPa and  $f_c=0.05$  were assumed in the calculations. Figures 2 and 3 compare the computations and the experimental results. It shows that, with the Rousselier model, a perfect correlation can be obtained with  $f_0=2E-5$ . The predicted diameter reduction at the onset of rupture is 2.5 mm, which represents 5% difference in comparison to the experimental rupture point. A similar analysis was performed with the GTN model. The results show that if nucleation is accounted for,  $f_0=2E-3$  or  $f_0=2E-5$  gives results in very good agreement with the experimental data. In contrast, if nucleation is not accounted for, only the results obtained with  $f_0=2E-3$  allow to reproduce the observed experimental values at fracture. These results suggest that the 2 models use a different definition of the initial void volume fraction.

In a previous study, carried out within Phase 1 of this Round Robin [2], a similar result was obtained and it was concluded that using the Rousselier model, the initial void volume fraction was probably less than suggested in the Round Robin. This was confirmed by Keim from Siemens KWU, Germany, whom indicated that the material used for the ESIS TC8 Phase I Round Robin was identical to that used in another Round Robin for which the chemical composition of the 22 NiMoCr 3 7 was available. Franklin's formulae gives  $f_0=1.5E-4$  which is approximately 10 times lower than the  $f_0$  value proposed in this Round Robin and better corresponds to the value identified with the Rousselier model. When using the GTN model with nucleation, the initial void volume fraction no longer influences the results. It is therefore concluded that the discrepancy observed between the two models arises from the fact that nucleation has a major influence with that particular material. This is not accounted for in the Rousselier model but decreasing the initial void volume fraction improves the predictions.

With the identified critical damage parameters, the two models allow to predict well the behaviour of the specimen observed experimentally. The predicted diametrical contraction as a function of elongation is compared to the experimental one in Figure 4. The predictions obtained with the Rousselier model better matches the experimental data than with the GTN model. Also reported on this Figure is the volume conservation law expressed as  $\Delta D = D_0(1 - \sqrt{1/(1 + \Delta L/L_0)})$ . It shows that as necking occurs, the volume conservation law no longer prevails. Note also that it occurs after the maximum load.

## NUMERICAL SIMULATION OF A COMPACT TENSION SPECIMEN

The mesh used for the computation of the 20% side grooved CT25 specimen follows the Round Robin specifications : due to the symmetries, only a 2D plane strain calculation of one half of the specimen can be performed. The mesh is constituted of 3040 isoparametric quadratic 8 nodes elements with 4 Gauss points and 9353 nodes. In the ligament, 54 elements are used with a length  $l_x=0.1$  mm and an height  $l_y=0.2$  mm, as requested in the Round Robin. The loading is simulated as a vertical nodal displacement of the load point.

The crack extension is calculated using a post-processing procedure which consists in comparing, at each load step and for the Gauss points of the elements in the ligament, the value of  $f$  to  $f_c$ . As a Gauss point of an element reaches the critical void volume fraction, one half of the element length is considered to be damaged. The J-integral values are calculated using a virtual crack extension method available in CASTEM 2000. It is well known that for fracture mechanics coupled damage calculations, the J-integral is path dependent and the largest contour is required to obtain J value comparable to that determined experimentally.

For the sake of completeness, the results obtained with the Rousselier model and the damage parameters specified in the Round Robin ( $f_0=2E-3$ ,  $l_x=0.1$ mm and  $l_y=0.2$  mm) are compared with the experimental values in Figures 5 and 6. Clearly, these parameters do not allow to reproduce the observations. Further simulations were then conducted to identify the correct value of  $L_c$ . Naturally, the value of  $f_0$  identified with

the smooth tensile specimen was assumed. As already stated in the identification procedure, unless there is metallographic evidences that show different distributions of inclusions in perpendicular orientations, it is recommended to use square elements to model the crack growth path. Consequently, for that Round Robin, square elements were adopted and the best correlation between the computations and the experimental data was obtained for 0.45mm square elements.

Some of the results obtained with the GTN are also shown in these Figures. As for the Rousselier model, the best results are obtained assuming void nucleation, the identified value of  $f_0$  and 0.45mm square elements. All the other options that were tested (and in particular using that model without nucleation as specified in the Round Robin) did not allow to obtain satisfactory results.

## DISCUSSION

Data obtained from a smooth tensile specimen was available in the Round Robin to identify  $f_0$ . Clearly, these specimens can be used but are not the most suitable to perform such an identification. The prediction of the post-necking behaviour is difficult to achieve and highly dependent upon the large strain algorithm used in the code. In addition, from an experimental point of view, the position of the diametrical extensometer along the length of the specimen at the location of necking presents one further technical difficulty. It also requires the use of a small imperfection which is known to substantially influence the predictions [2].

Concerning the identification of  $L_c$ , it is often recommended to use an effective thickness  $B_{eff} = \sqrt{B \cdot B_n}$  to account for the influence of side grooves. In this Round Robin, it has been observed that a perfect correlation between the calculation and the experimental data was obtained using the net thickness instead of the effective thickness. This will have to be addressed in more detail in the future.

Finally, a comparison of the  $J$  values at initiation ( $J_i$ ) with the predictions was achieved. One reliable way for determining this value is to examine the width of the stretched zone at the onset of crack extension [11, 12]. Since this value was not available in the Round Robin, it was determined from an analysis of the  $J_R$  curve. The tearing resistance curve was first extrapolated to a 0 value of crack extension, as shown in Figure 7.  $J_{i\_exp}$  was then determined as the intersection between the extrapolated  $J_R$  curve and the blunting line as defined by Schwalbe et al. [13]. In this document, the blunting line is expressed by  $J=3.75 \cdot R_m \cdot \Delta a$  where  $R_m$  is the ultimate tensile stress. From the stress-strain curve of the material given in the Round Robin, the blunting line is then expressed by  $J=2336 \cdot \Delta a$ . The intersection between the  $J_R$  curve and the blunting line gives  $J_{i\_exp}=229$  N/mm and  $a_{i\_exp}=0.1$  mm. A comparison of the predicted  $J_i$  values for all the calculations is given Table 1. For both models, the best agreement is obtained with  $f_0=2.0E-5$  and 0.45mm square elements, that is the identified damage parameters.

## CONCLUSIONS

This 2<sup>nd</sup> phase Round Robin organised within the ESIS TC8 committee was one further opportunity to validate CEA's ductile critical damage parameter identification procedure. Both the Rousselier and the Gurson-Tveergard and Needleman model damage parameters have been successfully identified from a comparison between calculated and experimental smooth tensile and compact tension tests data.

Using the Rousselier model, it has been shown that the initial void volume fraction proposed in the Round Robin is likely to be too high. With this model, a good correlation between the load versus  $V_{LL}$  curve and the  $J_R$  curve was obtained with  $f_0=2.0E-5$  and  $L_c=0.45$  mm. Provided that void nucleation was accounted for, similar results could be obtained with the GTN model.  $J$  values at initiation compared favourably with the experimental data. It is concluded that the identification procedure has reach such a level of confidence that it can be used to draft an ESIS recommendation applicable to cracked bodies.

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## TABLES

**Table 1** : Calculated CT characteristics at initiation

Model	Void nucleation	Initial void volume fraction $f_0$	Element size ( $L_x$ $L_y$ ) (mm)	$V_{LL}$ (mm)	Load (kN)	$\Delta a$ (mm)	$J_i$ (N/mm)	$(J_i - J_{i\_exp})/J_i$
Rousselier	N	2E-3	0.10 0.20	0.74	51.7	0.050	120.5	-0.474
Rousselier	N	2E-5	0.10 0.20	0.59	50.3	0.050	72.4	-0.684
Rousselier	N	2E-5	0.30 0.30	0.71	52.1	0.150	106.9	-0.533
Rousselier	N	2E-5	0.45 0.45	0.88	52.7	0.225	148.2	-0.353
GTN	N	2E-3	0.10 0.20	1.03	51.9	0.050	175.3	-0.234
GTN	N	2E-5	0.10 0.20	1.41	56.8	0.050	276.0	0.205
GTN	N	2E-3	0.45 0.45	0.89	51.4	0.225	149.1	-0.349
GTN	N	2E-5	0.45 0.45	1.65	56.7	0.225	350.4	0.530
GTN	Y	2E-3	0.10 0.20	0.90	51.3	0.050	145.2	-0.366
GTN	Y	2E-5	0.10 0.20	1.05	54.3	0.050	182.0	-0.205
GTN	Y	2E-3	0.45 0.45	0.89	51.3	0.225	149.1	-0.349
GTN	Y	2E-5	0.45 0.45	1.16	53.6	0.225	217.5	-0.050

