MODELS OF CRACK INITIATION AND PROPAGATION THROUGH THE FINITE ELEMENT METHOD FOR THE EVALUATION OF THE ZR-2.5%NB ALLOY PRESSURE TUBES FRACTURE TOUGHNESS

VASILE RADU, LIVIA STOICA, ALEXANDRA JINGA, MIRELA MATEI, DENISA TOMA, VALENTIN OLARU

Institute for Nuclear Research (RATEN ICN) Pitești, Romania
e-mail: vasile.radu@nuclear.ro

Abstract

CANDU reactor uses Zr-2.5%Nb alloy pressure tubes as the primary coolant containment. Modelling the fracture toughness of the CANDU pressure tube, Zr-2.5%Nb alloy plays a very important role in the structural integrity analysis of the CANDU fuel channel, because all the failure criteria involved in cracking induced by the hydrogen up-take of the Zr-2.5%Nb alloy (DHC phenomenon) are based on the K_{IC} or J_{IC} fracture mechanics parameters. The objective of the work is to perform comparative analyses regarding the initiation and propagation of cracks in a Compact-Tension (CT) sample, made with the finite element method using three models: Crack growth through the extinction of finite elements (Gurson-Tvergaard-Needleman Model), Cohesive element model, Finite element mesh node release model. To evaluate the performance of each crack initiation and propagation model, a comparison is made with the values obtained in references from the specialized literature and the works carried out within the Fuel Channel CD Program.

Keywords: *CANDU pressure tube, fracture toughness, Crack initiation, Crack propagation*

Introduction

The pressure tubes made of 2.5%Nb alloy are the critical components of the CANDU fuel channels, due to the severe operating conditions during reactor life. The internal pressure of the cooling agent is about 10 MPa and the temperature varies in a range from 250 °C (at the entrance of the cooling agent into the pressure tube) and up to approximately 310 °C (at the exit of the cooling agent through the opposite end).These tubes are subjected to a total fast neutron flux of $3 \cdot 10^{26}$ n/cm^2 (for a life time of about 30 years, as estimated for CANDU 6, and to a permanent absorption of deuterium after a slow corrosion process [1].

In essence, the phenomena of degradation over time of the pressure tubes are a consequence of the simultaneous exposure to high mechanical stresses, high temperatures and fast neutron flow, a fact that leads to the substantial modification of the material properties. The phenomenon of slow crack propagation in the hydrated state and under mechanical tension (DHC - Delayed Hydride Cracking) [2], which is specific to pressure tubes made of zirconium alloys, is given special attention in the CAN-CSA N285.8-2021 standard [3]. The research programs that take place within Canadian profile organizations [4] highlight specific objectives related to nuclear security.

One of the material properties with a great influence on the operational safety of the CANDU pressure tube, made from the Zr-2.5%Nb alloy, is the fracture toughness. This material property can be adequately described by two fracture mechanics parameters, namely the critical intensity factor of the mechanical stress, K_{IC}, and the integral J_{IC}. There is one more property that describes the resistance capacity of the material to the propagation of a crack, namely the J - R curve. It should be mentioned that the Zr-2.5%Nb alloy has a high tenacity when installing the pressure tubes in the CANDU reactor, due to the fact that the alloy is ductile and contains a small amount of dissolved hydrogen. As the operating and stationary time in the reactor increases, the fracture toughness changes, being influenced by deuterium absorption through the corrosion phenomenon and by the effects of prolonged irradiation.

In the Canadian literature, special efforts are made to develop a model of the toughness of the Zr-2.5%Nb alloy, which takes into account the previously mentioned variables. The importance of the parameter that defines the toughness at break is also given by the fact that the Leak-Before-Break argument, which defines the ability to detect coolant leaks before the crack has an unstable propagation, is based on the toughness of the material, represented in this case of integral J_{IC}.

In the framework of the Fuel Channel Research Program, an experimental and modelling program is being carried out regarding the toughness of the Zr-2.5%Nb alloy from which the CANDU pressure tube is made. In this paper, the facilities of the FEACrack fracture mechanics software are exploited, which is a finite element analysis program for structures with cracks.

FEACrack™ fracture mechanics software is a 3D crack analysis program using the finite element method with automatic discretization generation [5]. It has available both the elastic analysis options for the mechanical stress intensity factor, *K*, and for the analysis in the elastic-plastic field, where the relevant fracture mechanics parameter is represented by the *J* integral.

Models for crack initiation and growth in ductile materials

Within the analysis options of the FEACrack program for the initiation and propagation of a crack, three options are available, namely:

- "Cell Crack Mesh for Element Extinction Crack Growth" option, (Gurson-Tvergaard-Needleman model);
- "Cell Crack Mesh for Cohesive Element Crack Growth" option;
- "Cell Crack Mesh for Node Release Crack Growth" option.

All the above mentioned options will be analyzed on the Compact Tension sample to obtain the *J - R* resistance curve, and subsequently the fracture toughness shown by the J_{IC} parameter.

The Gurson-Tvergaard-Needleman model for the study of crack growth in ductile materials

Gurson first proposed [6] a flow potential type function for porous materials. The "flow potential" type function was determined using unit cell studies having a concentric spherical void. The macroscopic flow potential for a porous material has been described in terms of void volume fraction *(f)*, which is the ratio of void volume to unit cell volume. The Gurson flow potential depends on the hydrostatic stress, in contrast to the von Mises flow potential, which is independent of the hydrostatic stress.

Using bifurcation localization studies, Tvegaard modified the Gurson model to take into account the interaction of micro-gaps, introducing three interaction parameters: q_1=1.5, q_2=1.0, q_3=2.25. Finally, Tvergaard and Needleman modified the Gurson criterion to take into account the rapid loss of mechanical load-bearing capacity during the void coalescence phase. For this, the void growth rate is accelerated after a certain value of the void fraction, which is called the critical volume fraction of voids, f_C. This last form of the model is the most popular and is known as the "GTN model", being used in the simulation of ductile fracture in metals.

The GTN plastic potential has the form [5]:

$$\Phi\left(\sigma_e,\sigma_h,f^*,\sigma_y\right)=\left(\frac{\sigma_e}{\sigma_y}\right)^2+2\cdot f^*\cdot q_1\cdot\cosh\left(q_2,\frac{3}{2},\frac{\sigma_h}{\sigma_y}\right)- \\ -\left[1+q_3\cdot\left(f^*\right)^2\right]=0 \quad (1)$$

with:

σ_e – effective stress (von Mises);

σ_h – hydrostatic stress;

$\sigma_y=\sigma_y\left(\varepsilon_{eff}^p\right)$ - the yield stress in the curve of the material, defined in terms of effective plastic deformation ε_{eff}^p;

f^* - volume fraction modified by voids.

The void growth acceleration mechanism is initiated when the volume fraction of voids, f^*, exceeds the critical volume fraction of voids, f_c. The void growth is amplified by a void growth acceleration factor, *K*, until the fracture void fraction value, f_F. The volume fraction modified by voids f^* in the GTN model has the expression:

$$f^*=\begin{cases} f & if \quad f\le f_c \\ f_c+K\left(f-f_c\right) & f_c<f<f_F \end{cases} \quad (2)$$

with:

$$K=\frac{\overline{f}_F-f_c}{f_F-f_c} \quad (3)$$

$$\overline{f}_F=q_1+\frac{\sqrt{q_1^2-q_3}}{q_3} \quad (4)$$

The change in the volume fraction of voids is due to the increase of existing voids as well as the appearance of new voids. Thus, the rate of change in the volume fraction of voids is expressed as a sum of the growth rate of the existing voids, $\dot{f}_G$, and the void nucleation rate, $\dot{f}_N$. Using conservation of mass, the rate of growth of existing voids is expressed in terms of hydrostatic plastic strain rate:

$$\dot{f}_G=(1-f)\cdot\dot{\varepsilon}^p \quad (5)$$

The void nucleation rate is considered proportional to the effective plastic deformation rate:

$$\dot{f}_N=A\cdot\dot{\varepsilon}_{ef}^p \quad (6)$$

$$\text{with } \dot{\varepsilon}_{ef}^p=\int_0^t\left\|\dot{\varepsilon}^p\right\|dt \quad (7)$$

and $\dot{\varepsilon}^p$ represents the plastic strain rate tensor.

A Gaussian distribution is used for the constant A:

$$A=\frac{f_N}{s_N\sqrt{2\pi}}\cdot\exp\left[-\frac{1}{2}\cdot\left(\frac{\dot{\varepsilon}_{ef}^p-\dot{\varepsilon}_N}{s_N}\right)^2\right] \quad (8)$$

with: ε_N represents the average nucleation strain having the standard deviation s_N, and f_N is the volume fraction of voids of voids that nucleate.

The GTN model has nine parameters, which require an adequate calibration in order to apply the model concretely to a ductile deformation and fracture process. Together with these parameters, the following relationship is required:

$$\sigma_y=\sigma_y(\varepsilon_{ef}^p) \quad (9)$$

In this way the description of the model is complete. For the 3D WARP solver [7] of the FEACrack software, within this damage model, element failure occurs when the current void fraction, f, reaches a user-specified critical value, f_C. The current implementation of the GTN model limits the "fracture" condition to a critical void fraction independent of triaxiality. Typical values of f_C for structural steels and pressure vessels are 0.1-0.25, compared to initial void fractions, f_0=0.0005-0.005.

The model of the cohesive zone used to study the growth of a crack in ductile materials

The concept of cohesion zone [8] was originally conceived by Dugdale in 1960 [9], Barenblatt in 1962 [10], Rice in 1968 [11] and other researchers in the following years. This concept considers that rupture is a gradual phenomenon in which separation occurs between two adjacent virtual surfaces through an extended crack tip (cohesion zone) and its propagation takes into account the presence of cohesive forces.

This fracture theory led to a new numerical approach for the simulation and study of crack propagation. In this approach, the continuum is characterized by two constitutive relations:
(i) A volumetric constitutive model describing the "bulk behaviour" of the material;
(ii) A cohesive surface constitutive relationship between tension and displacement that characterizes the behaviour of the interface surfaces between elements.

It is considered a quasi-statically stressed solid sample with a crack on the surface. Along the potential path of crack propagation, a pair of virtual crack surfaces is assumed, which are subjected to a separation force called de-cohesion tensile force. Based on the principle of virtual work and considering the contribution of cohesive traction, the balance equation can be expressed as follows:

$$\int_V \vec{s} : \delta\vec{F} dV - \int_{S_{\text{int}}} \vec{T}_{CZ} \cdot \delta\vec{\Delta} dS = \int_{S_{\text{ext}}} \vec{T}_{ext} \cdot \delta\vec{u} dS \quad (10)$$

with

V – sample volume;

S_{int} – cohesive internal surface;

S_{ext} – external surface;

$\vec{s}$ – the nominal stress tensor, $s = F^{-1}det(F)\sigma$, where $\vec{F}$ is the deformation gradient and σ is the Cauchy mechanical stress;

$\vec{T}_{CZ}$ – the cohesive traction vector, $\vec{T}_{ext}$ is the external traction vector;

$\vec{u}$ – the displacement vector, $\vec{\Delta} = u^+ + u^-$ – displacement between two adjacent cohesive surfaces;

$\vec{\Delta}$ – the relative displacement vector or separation vector.

The cohesive surface contribution is described by the integration term over the internal surface $\int_{S_{\text{int}}} \vec{T}_{CZ} \cdot \delta\vec{\Delta} dS$.

For isothermal conditions, the traction vector acting on the cohesive surface $\vec{T}_{CZ}$, simplified as $\vec{T}$, can be obtained by deriving the interfacial potential $\phi(\vec{\Delta})$:

$$\vec{T} = \frac{\partial\phi(\vec{\Delta})}{\partial\vec{\Delta}} \quad (11)$$

with: $\phi(\vec{\Delta})$ free energy density function per unit undeformed area.

By the appropriate selection of the potential function ϕ, the constitutive equations between cohesive traction and relative separation can be formulated. Various forms of the potential have been proposed in the literature, such as the linear, bilinear, polynomial or exponential form. For computations using the finite element method, the exponential form of the potential free energy density [8] is more convenient.

3D WARP finite element mesh node release model for crack growth in a material

In the WARP 3D solver [7], there is an option regarding crack growth analysis by releasing the nodes of the finite element network, setting some failure criteria. In this type of crack growth, called *node_release*, an increase in crack extension on a plane of symmetry is achieved by a traditional node release procedure. When the growth conditions are met, the displacement constraint holding the crack closed at that point on the front is replaced by the corresponding reaction force, which is then relaxed to zero.

The force release process occurs over a user-specified number of steps or using a pull separation pattern. The element remains in the model and most undergo inelastic unloading and then yielding as the crack tip continues to extend. Node release procedures support crack growth along multiple crack fronts on the plane of symmetry and easily model non-uniform growth along the front, for example through the "tunneling" effect. Currently, growth conditions are specified by a critical crack tip opening displacement angle (Crack Tip Opening Displacement - CTOA). The growth processor examines each possible CTOA value using element edges incident on an active front node and grows the crack when any of these angles exceeds the specified critical value. The user can also request crack extensions during the analysis, regardless of the crack growth criterion.

In the finite element method, strategies for releasing nodes generally follow one of the following two approaches:

1) user-specified external loads and displacement boundary conditions remain fixed, while additional loading steps relax the reaction forces to zero on the newly unconstrained nodes;

2) the loads and displacement boundary conditions continue to change to user-specified values during subsequent loading steps, concurrently with the relaxation of the reaction forces on the newly unconstrained crack front nodes.

The WARP 3D solver adopts the second strategy for two reasons:

a) models more closely the physical process of crack growth, thus minimizing the effects of artificial elastic unloading of the material;

b) computation time is dramatically reduced by eliminating additional "release" steps. Numerical studies reveal negligible differences in solutions with the two strategies.

Results of analyses by finite element analysis

In the three analyses for the considered CT sample, the requirements stipulated in the ASTM E1820 [12] standard for mechanical stress and dimensioning were taken into account. At the same time, the method of calculating the integral *J* was taken into account, which for an increase of the crack by 2 mm, represents the fracture mechanics parameter J_{IC}. In order to evaluate the performances of each crack initiation and propagation model, a comparison of the values obtained in each of the mentioned analyses for the integral *J* with the values obtained in the Canadian reference [13]. It should be mentioned that the material properties are taken for the Zr-2.5%Nb alloy from the CAN/CSA N285.8-21 standard [3], and the Ramberg – Osgood form was used for the constitutive equation.

Results from the Gurson-Tvergaard-Needleman model

The first analysis performed with the fracture mechanics software FEACrack is the "Cell Crack Mesh for Element Extinction Crack Growth" option, which is based on the Gurson-Tvergaard-Needleman (GTN) model. After running the FEACrack analysis, this option allows the visualization of the crack advance front, depending on the mechanical stress step. Thus, in Fig. 1, the area of crack propagation at the loading step 100 is represented.

Figure 2 presents the results of the FEACrack computations for the CT sample made of the Zr-2.5%Nb alloy.

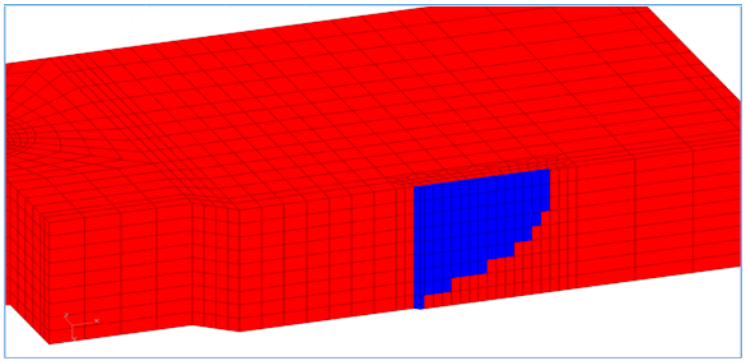


Fig.1. Crack propagation surface at load step 100, described by the extinction of the elements in GTN model ("killed status" analysis parameter)

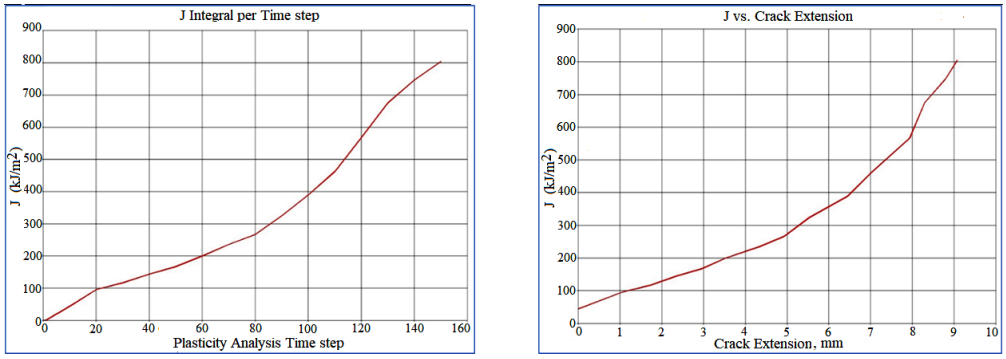


Fig.2. FEACrack computations for the CT sample made from the Zr-2.5%Nb alloy (GTN model): dependence of integral J on plasticity time step (left) and the J-R curve (right)

From the analysis of the *J-R* curve obtained with FEACrack for the CT sample made of the Zr-2.5%Nb alloy (Fig. 2), it can be found that for a crack propagation $\Delta a = 2$ *mm*, a value of the *J* integral corresponds to approximately: $J = 130$ kJ/m^2. This value was compared with those obtained in reference [13] within the experimental tests performed on CT samples made of Zr-2.5%Nb alloy, with a nominal hydrogen content. Thus, for the integral *J* values obtained at the maximum load, J_{ml}, which are considered representative for the type of CT sample that can be made from the CANDU pressure tube, the range obtained in [13] was: J_{ml}=128.3-130.3 kJ/m^2.

The results from the model of the cohesive zone

The second analysis performed with the fracture mechanics software FEACrack is the "Cell Crack Mesh for Cohesive Element Crack Growth" option, which is based on the model of the cohesive elements model. Figure 3 shows the dependence of the integral *J* from the crack tip on the time step of the plasticity analysis and *J-R* curve.

From the analysis of the J-R curve obtained with FEACrack for the CT sample made of Zr-2.5%Nb alloy, it can be found that for a crack propagation $\Delta a = 2$ *mm*, a value of the *J* integral corresponds to approximately: $J = 94$ kJ/m^2.

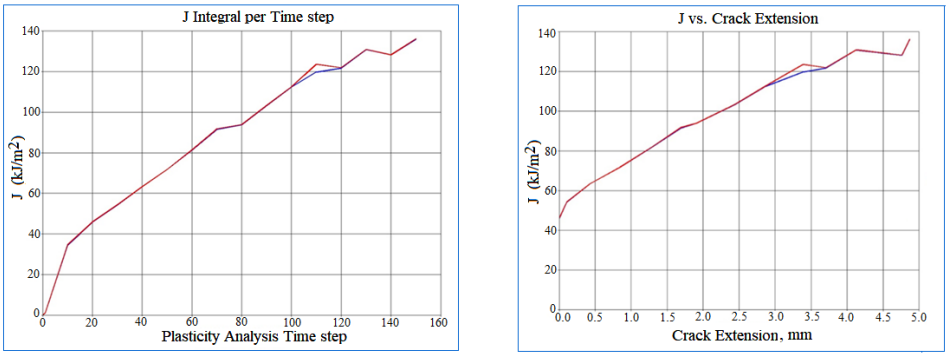


Fig. 3. FEACrack computations for the CT sample made from the Zr-2.5%Nb alloy (Cohesion zone model): dependence of integral J on plasticity time step (left) and the J-R curve (right)

The results from the model of the node release

The third analysis performed with the fracture mechanics software FEACrack is the "Cell Crack Mesh for Node Release Crack Growth" option, which is based on the node release model. Figure 4 presents the *J-R* curve obtained with FEACrack for the CT sample made of Zr-2.5%Nb alloy.

From the analysis of the J-R curve, under the elastic analysis conditions specific to this model, it can be found that for a crack propagation $\Delta a = 2$ *mm*, a value of the *J* integral corresponds to approximately: $J = 240$ kJ/m^2.

It is found that the analysis performed using the FEACrack software with the "Cell Crack Mesh for Node Release Crack Growth" option, which is based on the node release model, gives results which are not consistent with those obtained in reference [12].

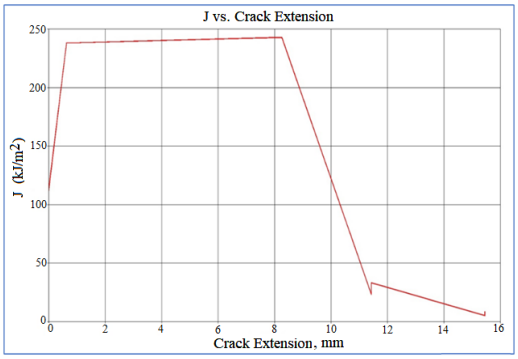


Fig. 4. The J-R curve obtained with FEACrack for the CT sample made from the Zr-2.5%Nb alloy (Node release model)

Conclusions

In the three analyzes for the considered CT sample, the requirements stipulated in the ASTM E1820 standard for mechanical stress and dimensioning were taken into account.

At the same time, the method of calculating the integral *J* was considered, which for an increase of the crack by 2 mm, reproduces the fracture mechanics parameter J_{IC}.

In order to evaluate the performances of each crack initiation and propagation model, a comparison of the values obtained in each of the mentioned analyzes for the integral *J* with the values obtained in the Canadian reference was made.

It should be mentioned that the material properties for the Zr-2.5%Nb alloy are taken from the CAN/CSA N285.8-2021 standard, and the Ramberg – Osgood form was used for the constitutive equation.

The integral *J* values obtained at the maximum load, J_{ml}, which are considered representative for the type of CT sample that can be made from the CANDU pressure tube, were in the range: $J_{ml} = 128.3$-130.3 kJ/m^2.

From the analysis of the *J-R* curve obtained with FEACrack for the CT sample made of the Zr-2.5%Nb alloy, it can be found that for a crack propagation Δa=2 mm, the values of the *J* integral correspond to approximately:
- $J = 130$ kJ/m^2, with GTN model;
- $J = 94$ kJ/m^2, with the cohesive zone model;
- $J = 240$ kJ/m^2, with the node release model.

As a general conclusion, the analysis performed with the FEACrack software with the "Cell Crack Mesh for Element Extinction Crack Growth" option and with the model described by the input parameters established in the paper gave the best results in very good agreement with the experimental results.

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