Finite Element Prediction of Endcap Stresses Under Accident Conditions

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ABSTRACT

This paper is concerned with a two-dimensional finite element-based simulation of thermal and mechanical responses of a nuclear fuel element under accident conditions, such as large break LOCA and fast LOR. Comparing with the standard 1D-based analyses utilized by the nuclear industry, the present 2D analysis provided the possibility for detailed assessment of stresses and failures in the endcap region during the accident transients. To improve efficiency and stability of computations, a special computational strategy was developed based on the VAST suite of nonlinear finite element programs. The material properties of fuel and sheath/endcap materials were identified from the database. Representative time-dependent power pulse and boundary conditions for accidents were employed. Transient temperature and stress/strain fields in and around the endcap region were predicted and associated with the relevant failure criteria.

INTRODUCTION

Constrained axial expansion of the fuel string within a CANDU fuel channel is typically associated with fuel heatup after a large break Loss-of-Coolant Accident (LOCA) or a fast Loss-of-Regulation (LOR) event. All utilities have mitigated the potential for fuel axial compression by ensuring that there is sufficient axial clearance in the fuel channel to accommodate the axial expansion of the fuel string. However, the same mechanisms can also create large axial stresses in the fuel elements that may lead to sheath or end cap failures.

The Canadian nuclear industry standard code for modelling fuel behaviour during normal operation is based on a finite element variant of the ELESIM code, named ELESTRES [1]. These codes represent the physical phenomena using an axi-symmetric model of a fuel element (i.e., a plane through the fuel element centreline). The fuel region is modelled in detail where the cross-section of the fuel stack is divided into 100 annuli for temperature calculations. Changes in fuel microstructure, fission product gas release, internal gas pressure, fuel-to-sheath heat transfer coefficient plus a host of other slowly varying phenomena are included.

The Canadian nuclear industry standard code for modeling fuel behavior for an accident scenario, such as a large break LOCA or a fast LOR is 1D program named ELOCA. This is a companion code to ELESTRES, which obtains fuel condition at the start of an accident simulation from an ELESTRES output file, named ELDAT. The sheath behavior is modeled in detail, including radial and axial contacts and thermo visco-plastic deformations [2]. A large number of sheath failures mechanisms, such as low-ductility athermal strain failures, beryllium assisted crack penetration, oxide layer cracking with localized strain failure, sheath embrittlement, fuel melting and sheath melting, are all considered in the ELOCA code.

The current version of ELOCA predicts when the endcaps are put under stress by axial expansion of the fuel stack. However, due to the 1D nature of the program, detailed endcap models are not considered. The purpose of the present study was to perform a 2D axisymmetric numerical simulation to assess the stresses and strains in the vicinity of the endcap under various accident conditions and associate them with the endcap failure criteria. In these analyses, detailed geometric and material properties of the endcap were included.

The 2D numerical simulations considered in the present work required steady state and transient solutions to a coupled nonlinear thermal-mechanical problem. The nonlinearity involved in this problem was not only associated with the microstructure-based thermo-viscoplastic model that represented the high temperature behavior of the Zircaloy material, but also due to the thermal and mechanical interactions between the fuel stack and the sheath/endcap assembly. In the present study, a reliable and efficient finite element-based computational procedure was developed for these analyses based on the VAST suite of general-purpose nonlinear finite element codes that was developed and maintained by Martec Limited over the last three decades [3].

After the development of the computational procedure, some preparatory tasks must still be performed before the actual analyses can take place. These included collection and verification of the fuel and sheath material properties over the temperature range of interest, preparation and verification of the finite element analysis tools and determination of the input thermal loads and initial/boundary conditions for selected transient accident conditions. All these issues will be addressed in the following sections, which will be followed by presentations of results and discussions of the 2D finite element simulations of the fuel element under various accident conditions. Conclusions will be presented at the end of the paper.

DEVELOPMENT OF COMPUTATIONAL STRATEGY

As mentioned before, accurate solutions to the thermal and mechanical responses of fuel elements under transient accident conditions required fully coupled heat transfer-stress analyses. This is because the heat transfer properties at the fuel-sheath and fuel-endcap interfaces are strongly influenced by the contact conditions in those areas, and on the other hand, the thermal-strain-induced contact conditions over these interfaces are controlled by the local temperature distributions. However, these fully coupled analyses are often time-consuming and sometimes unstable. Fortunately, the ELOCA program has been developed which is able to calculate the time history of the heat transfer coefficient at the fuel-sheath interface during the entire period of the accident. When this interface heat transfer coefficient was adopted in the 2D finite element simulations, the present analysis became one-way coupled, in which the heat transfer problem could be solved completely independent of the mechanical deformations, and the resulted transient temperature field could then be applied to the stress analysis model to compute the thermal-strain-induced stresses in all structural components. Based on this consideration, a more reliable and efficient computational procedure was developed in the present work for the 2D transient finite element simulations. This procedure involved two distinct finite element models as will be described below.

Model I was for steady state and transient heat transfer analyses of the complete fuel element, including both the fuel stack and the sheath/endcap assembly. Time histories of thermal loading, interface conductance between the fuel-to-sheath and sheath-to-coolant interfaces, and the coolant temperature were specified. The non-uniform radial and axial distributions of the energy release rate were also considered in this model. Prior to the transient heat transfer analysis, a steady state analysis was performed using the normal operation conditions to generate the initial conditions.

Model II was for static and transient stress analyses of the fuel stack and sheath/endcap. Temperature distributions resulting from the solutions of *Model I* were prescribed to this model to obtain thermal expansion strains. The outer boundary of this model was exposed to the coolant pressure, whereas the internal gas pressure and gap elements were applied to the fuel/sheath and fuel/endcap interfaces.

In addition to the standard capabilities of axi-symmetric solid elements as provided in most of the general-purpose finite element program, such as VAST [3], some specialized features were required in the present numerical simulations. These features include (a) a thermo-viscoplastic model for representing the temperature-dependent, nonlinear mechanical behavior of the Zircaloy-4 at elevated temperatures; (b) a special interface heat transfer element to describe the heat transfer across the fuel-sheath and fuel-endcap interfaces; (c) a gap element that is able to identify the contact-release condition automatically during a transient nonlinear simulation. Besides the analysis capabilities mentioned above, capabilities for considering temperature-dependent material properties and time-dependent boundary condition data are also required in the present simulations.

In the present study, the above-mentioned 2D computational procedure was implemented in the VAST suite of finite element programs [3]. The VAST suite is a general-purpose nonlinear finite element package, in which VASTF can perform nonlinear steady state and transient heat transfer analyses, and the VAST code is specialized for nonlinear stress analyses. The present version of VAST and VASTF provide a wide selection of element types, such as beam, shell and solid elements, a large material library, including linear elastic, visco-elastic, elasto-plastic and visco-plastic material models with temperature dependency, and a large selection of nonlinear solution procedures, such as the displacement control method, the constant arc-length method and the orthogonal trajectory method. In order to verify and validate the VAST suite of programs effectively on a regular basis, an Auto tester system has been developed. The current library of test cases included over 400 example problems that were carefully selected to cover all element types and analysis options provided by the VAST program. Over the years, the reliability, accuracy and robustness of the VAST suite of programs were demonstrated by solving numerous real-world engineering problems successfully.

ENHANCEMENT AND VERIFICATION OF FINITE ELEMENT CODE

Fuel-Sheath Interaction in Heat Transfer Analyses

The description of heat transfer between the fuel stack and the sheath requires a special interface element, which related the temperature differences and heat fluxes between these two surfaces through the interface heat transfer coefficient, h. Following the standard finite element procedure, the temperature fields on the two surfaces of the interface element can be expressed in terms of the nodal temperature values and using the principle of virtual temperature, we obtain the effective thermal conductivity matrix for the interface element. In finite element analysis, these effective thermal conductivity matrices need to be assembled into the global conductivity matrix. For transient problems, the heat transfer coefficient in the above equation can be a function of time.

Following its derivation and implementation in the VASTF heat transfer program, this interface element was verified using a 1D version of the steady-state heat transfer problem in the fuel element. The geometric dimensions, material properties and heat generation rate were taken from Reference [4] and the present results were compared with the analytical

and numerical solutions published in [4]. Excellent agreement was obtained. Verification for the transient case was carried out using a set of initial and boundary conditions typical to LOCA conditions.

Fuel-Sheath Contact in Stress Analysis

The mechanical interactions at the fuel-sheath and fuel-endcap interfaces were treated using the gap element provided in the VAST finite element program. Definition of a gap element involves specification of a node pair, on the master and slave surfaces, respectively, and a unit vector describing the direction of the potential contact. The initial contact status of a gap element is fully determined by the initial coordinates of the two nodes in the gap element. During the nonlinear analysis, the current gap size is calculated repeated at the iteration level. If the gap is open, no contact stiffness is assigned. If the gap is closed, a large contact stiffness will be used to prevent penetration of the master surface into the body of the target.

For nonlinear analyses involving geometric and material nonlinearities, convergence criteria are required to terminate equilibrium iterations when a pre-set accuracy measure has been achieved. In VAST, several convergence criteria were implemented based on different solution parameters, such as displacements, incremental work and out-of-balance force. For contact problems involving gap elements, which are often referred as boundary nonlinearities, additional convergence criteria must be introduced to ensure that the (contact/no contact) status and the predicted contact forces of all gap elements are no longer changing at the end of an iteration. In order to verify the gap element, we considered contact between two curved beams. This classical test case for contact problems was considered previously [5, 6]. The present results are in good agreement with the published solutions.

Thermal Visco-Plastic Behavior of Zircaloy-4

In the present work, a thermo-viscoplastic material model was implemented into the VAST program to characterize the complicated mechanical behavior of Zircaloy-4 at high temperature. It has been known that over the temperature range of interest, the Zircaloy material may transform between four distinct phases, namely the as-received phase, the alpha-annealed phase, the beta-annealed phase and the beta phase [7]. Each material phase has a different microstructure and an independent set of internal variables. During a transient deformation process, the transformation between these phases is driven by the temperature-time history according to a set of material evolution laws.

As for all finite element programs that provide nonlinear material modeling capabilities, time integration of the material model must be carried out at all numerical integration points in the elements. Due to the extreme complexity of the present thermal visco-plastic model, a large number of solution variables need to be stored at the numerical integration point level, including stresses, phase fractions, internal stresses, grain sizes and the effective creep strain rate. These data were required for conducting the equilibrium iterations and for restarting the analysis if divergence occurred during the transient nonlinear solution process.

In the original form of the thermal visco-plastic model for Zircaloy-4, shear stresses and strains were not considered. This treatment is sufficient for 1D solutions of the fuel element, such as those provided by the ELOCA code. However, it becomes insufficient for the present 2D finite element analysis since the significant shear strains and stresses may occur in the endcap region. To resolve this difficulty, we extended the Hill's yield surface to include the contribution of the shear stresses. Due to the lack of experimental data for anisotropic plastic behavior, in this work, the plastic shear deformation has been assumed to be isotropic.

A number of numerical integration algorithms have been implemented, including both explicit and implicit schemes. For the implicit method, the tangent moduli matrix has been derived for tangent stiffness calculations. Generally speaking, the explicit integration method is more efficient computationally and more convenient to implement, but normally requires a smaller time step size to maintain numerical stability of the overall finite element calculations. On the other hand, the implicit integration method is more stable and accurate at the structural level, but difficult to implement and requires iterations at the numerical integration point level. An automatic time step adjustment algorithm was developed to ensure numerical stability. Interested readers should be referred to reference [8] for details.

In order to verify the thermal visco-plastic material model, we considered nonlinear deformations of a simply supported circular plate subjected to both thermal and mechanical loadings. The effects of the numerical integration algorithms (explicit vs. implicit) and the time step size on the finite element solutions were studies extensively. This verification suggested that the implicit algorithm should be utilized along with a time step size corresponding to maximum visco-plastic strain increment of 0.00002.

MATERIAL PROPERTIES FOR HEAT TRANSFER AND STRESS ANALYSES

The present 2D numerical simulation of the fuel element involves steady state and transient heat transfer analyses. Because very large temperature variations are considered in these simulations, over which the material properties vary considerably, the use of proper temperature-dependent material properties in the analyses became crucial.

The material properties required in heat transfer analyses included thermal conductivity and specific heat capacity of both the fuel (UO_2) and sheath/endcap (Zircaloy-4) materials. These properties used in the ELOCA program were identified in [7] and verified against material property data reported in independently published journal paper [4] and report [9], which contained data from the INSC and MATPRO databases, respectively. The variation of specific heat caused by phase change in Zircaloy-4 was included.

Because in the present problem we are mainly concerned with deformations of sheath and endcap during an accident transient due to excessive thermal expansion of the fuel, the most important properties for stress analyses are the coefficient of thermal expansion or equivalently the variation of thermal strains with temperature for both the fuel and the Zircaloy-4 materials. These properties were extracted from both the ELOCA manual [7] and MATPRO database [9] and verified by comparing to each other. It was interesting to note that the thermal expansion in Zircaloy-4 was anisotropic, which was further complicated by the thermal contraction that occurred during alpha-beta phase transition. In addition to the thermal strain expressions, the Young's moduli of the fuel and sheath/endcap materials are also highly temperature-dependent.

FINITE ELEMENT RESULTS

Construction of 2D Finite Element Mesh

Two basic assumptions were adopted in the present 2D analyses, namely at the beginning of the transient analysis: (1) no initial gap existed between fuel and sheath/endcap in both the radial and axial directions, and (2) there is no mechanical interaction between the fuel and sheath, so no initial contact stresses occurred.

Because the focus of the present 2D finite element analysis is to assess potential failures in the end cap region, detailed endcap geometry must be considered in the 2D finite element model. After a survey of the geometries of a number of real end cap structures, a "generic" endcap design was developed. Although this artificial design involved simplifications from the real designs, it preserved all the essential structural features of a real endcap.

A nonlinear 8-noded axi-symmetric solid element based on the total Lagrangian formulation was employed in the present analysis [10] and the finite element mesh is shown in Fig. 1. The fuel element was approximately 0.5m long, but due to symmetry, only half of it was directly modeled. The finite element models for heat transfer and stress analyses had exactly the same mesh layout, so that the nodal temperatures calculated by the former could be readily applied to the later to compute thermal-induced strains. For stress analysis, all elements representing the sheath and endcap material were defined as thermal visco-plastic. The Zircaloy-4 material was assumed to be initially in the *as-received* phase with an internal stress of 64MPa. This material setting was believed to also provide a good approximation of the beta-annealed material in the heat affected zone around the sheath-endcap interface, as this material was subjected to irradiation hardening with an internal stress of about the same amount.
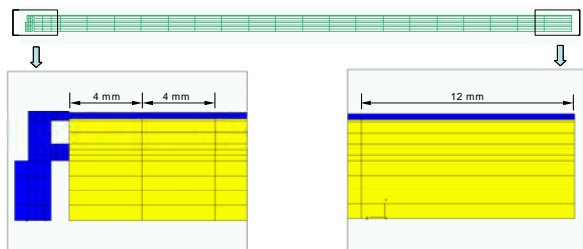

Fig.1: 2D Mesh of Fuel Element

The interface heat transfer elements and the gap elements were applied along the entire interface between the fuel stack and sheath/endcap in both the radial and axial directions. The fuel-to-sheath heat transfer coefficient required in the transient heat transfer analyses and the time history of internal gas pressure needed for stress analysis were both taken from ELOCA results. The contact/release conditions of gap elements were automatically adjusted during the analyses according to the relative displacements of the two nodes that define the gap element.

Simulation for Large Break LOCA Condition

The coolant conditions required for heat transfer and stress analyses of fuel elements included time histories of three physical quantities, namely coolant pressure, coolant temperature and coolant-to-sheath heat transfer coefficient. In order to describe the time history of the energy release rate, a scaling function must be applied to the power generation rate under normal operating conditions. In the present study, all these quantities were taken from a representative LOCA case.

Once the geometry and coolant/power pulse conditions were fully defined, we ran ELESTRES first to predict fuel/sheath conditions at the mid-span of the fuel element under normal operation condition conditions. In the ELESTRES run, we assumed a constant linear power output of 58 kW/m and a final burnup of 61 MW·h/kg U. Once the ELESTRES run was completed, the ELDAT file generated by ELESTRES was utilized, along with the coolant conditions and power pulse function represented earlier, to perform an ELOCA analysis. This ELOCA analysis produced time histories of internal gas pressure and fuel-to-sheath heat transfer coefficient, which were then utilized in the 2D heat transfer and stress analyses. In addition to being used as initial conditions for ELOCA analysis, the ELDAT file was also used to provide profile of radial

variation of the energy release rate from fuel. This information allowed us to accurately model power generation by the fuel in the 2D finite element analysis. The effect of end flux peaking was also considered.

In the 2D finite element simulations, a steady-state heat transfer analysis was first conducted to predict the temperature field under normal operation conditions. This temperature field was then utilized as the initial condition in a transient heat transfer analysis using the coolant conditions and power pulse function for the representative large break LOCA transient.
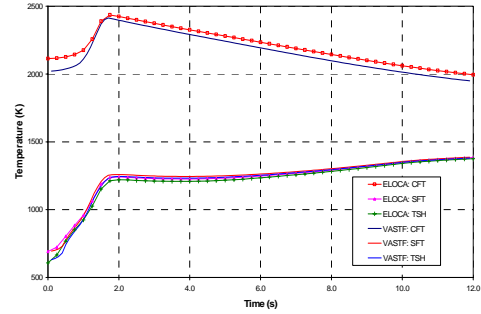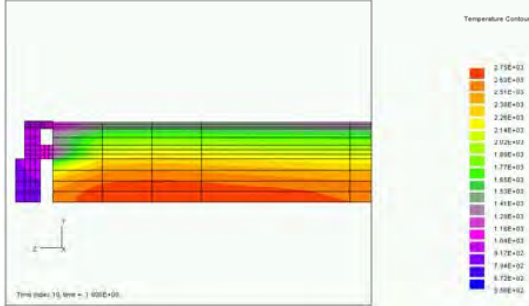

Fig. 2: Temperature Distribution During LOCA

Fig.3: Predicted Temperature Time Histories by VAST and ELOCA.

In order to get an idea about the temperature distribution in the end cap region at different times during the LOCA transient, a temperature contour plot was generated for times t=1.9s in Fig. 2. These temperature contours confirmed that the fuel stack was hotter towards the end due to end flux peaking, so the highest temperature in sheath occurred at a distance about 8mm from the sheath-end cap interface. The temperature time histories of the fuel center (CFT), the fuel surface (SFT) and the sheath (TSH) were reported in the ELOCA result file and were used to verify the results of the present transient finite element solutions using VASTF. The results obtained by both programs are compared in Figure 3. A very close agreement between these solutions is observed. Both programs predicted rapid temperature increases from the beginning of the LOCA transient until a peak temperature was reached at the fuel center at about t=1.9s.
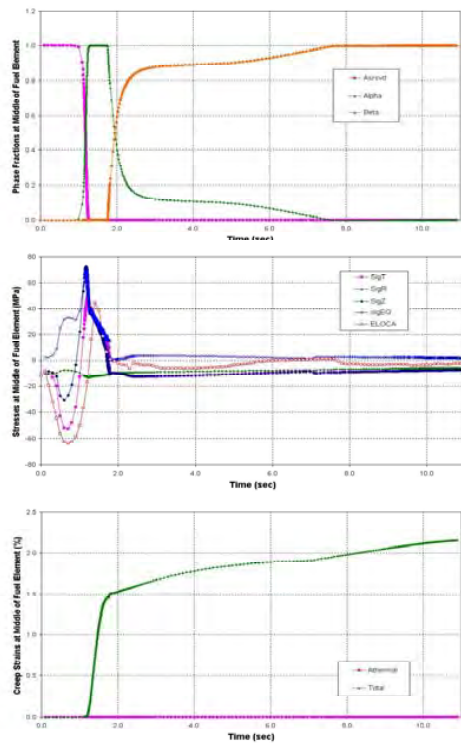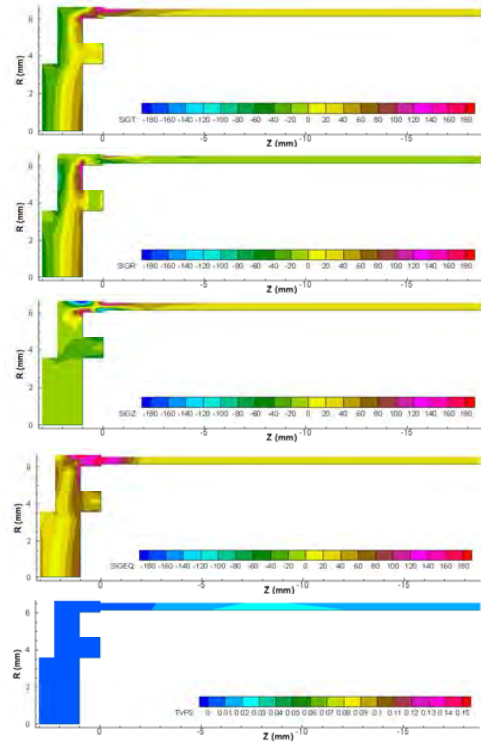

Fig. 4: Solutions at Mid-Span of Fuel Element.

Fig.5: Contour Plots for t=1.4s.

The advantage of the present 2D analyses lies in its ability to predict both radial and axial variations of the physical parameters of interest, including phase fractions, stress components, equivalent stress and the total and athermal creep strains, at each numerical integration point on the finite element model. The calculated time histories of different solution variables obtained at the mid-span of the sheath are given in Fig. 4 and the stress/strain distribution obtained at t=1.4s in the endcap area are shown in Fig. 5. In these figures, symbols "SigT", "SigR" and "SigZ" indicate the stresses in the circumferential (σ_θ), radial (σ_R) and axial (σ_Z) directions, respectively. "SigEQ" is the equivalent stress and "TVPS" the total visco-plastic strain. The time histories of stresses shown in Fig. 4 suggested that at the early part of the LOCA transient, the sheath expanded faster than the fuel, resulting in reduction of both the radial and axial contact stresses, which led to an increase of the compressive stresses in the sheath material before the development of significant tensile stresses. The hoop stress (σ_θ) time history predicted by ELOCA [2] is also shown in the figure for comparison purposes. A very reasonable correlation between the VAST and ELOCA solutions was obtained. A rapid increase of total creep strain was predicted between t=1.2s and 1.9s. After t=1.9s, the total creep strain continued to increase, but at a much slower rate. For the temperature range considered in these solutions, the total creep strain was dominated by the dislocation creep strain and the athermal strain was almost negligible. The contour plots indicated stress concentrations occurred at the corners in the endcap area.

Due to space limitations, the numerical results for the fast LOR accident condition were not included in this paper. The complete solutions are published in reference [8].

SUMMARY AND CONCLUSIONS

In this paper, we presented results from two-dimensional finite element simulations of the nuclear fuel element under large break LOCA and fast LOR conditions. These numerical simulations were performed based on a general-purpose finite element program, named VAST. The Canadian industry standard programs, ELESTRES and ELOCA, were also utilized in this study, not only to provide the fuel-to-sheath heat transfer interface conditions, but also to provide a means for partially verification of the present finite element results. Very good agreement between the ELOCA and VAST solutions was obtained whenever comparisons were possible.

For the LOCA case, the 2D finite element results indicated that the sheath strains are non-uniform along the length of the fuel element. The maximum creep strain in the sheath material reached 4.5% at a location about 8 mm away from the sheath-endcap junction. This was because higher temperatures occurred in this region due on the effect of end flux peaking. In addition, stress concentrations were also predicted at the corners of the sheath/endcap interface and the notch.

For the LOR case, the present finite element results indicated that in order to achieve the ELOCA-predicted initial compressive hoop stresses in the sheath, a small radial clearance must be included between the sheath and fuel stack in the finite element model. VAST predicted failure from high athermal strains at the corners of the sheath/endcap junction and around the notch in the endcap region. This was due to the fact that the majority of the thermal-induced axial load from the fuel stack was transferred to the endcap.

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