First steps toward a mechanistic model for core disassembly in a CANDU reactor

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(Dated: April 9, 2008)

Severe core damage accidents and core disassembly in CANDU reactors are areas of recent research efforts. In this paper a critical review is presented about the experimental and computational work related to these topics. The main properties of the relevant material are reviewed, keeping in mind their importance for any future attempt to simulate these processes from the computational point of view. Some ideas related with the physical processes relevant to the study of the core disassembly are addressed.

I. INTRODUCTION

In a CANDU reactor the two independent shutdown systems (SDS1 and SDS2) are designed to guarantee the fast shutdown of the reactor in the event of any failure. Once the reactor is shutdown, the potential for damage leading to releases of fission products will strongly depend on the engineered capacity to remove the decay heat (usually of the order of 3% FP). After reactor trip if the boundaries of the heat transport system (HTS) are intact then the joint action of the shutdown cooling system and the heat removal capability of the steam generator (SG) acting as a heat sink are enough to reject the heat from the fuel. In the case of loss of coolant accident (LOCA), then the joint action of the Emergency Core Cooling System (ECCS) and the SG are in most cases sufficient to deal with the removal of the decay heat. Additionally the moderator provides another effective heatsink for the generated decay heat. These systems are effective in preventing the progression of the consequences in a wide range of failure events.

Particular importance is devoted to the accidents included in the severe accident category. A severe accident is defined as one where the engineered systems are insufficient to remove the heat generated in the fuel for a large period of time, this class of accidents could lead to severe damage of the fuel and/or severe core damage including the possibility of core disassembly [1]. Two examples of the initiated events that can progress into a severe accident are those related with LOCA/LOECCS (loss of ECCS) and loss of multiple heat sinks [1, 2].

The project presented in this paper will focus on the analysis of the thermo-mechanical deformations of the fuel channels under severe core damage accident conditions. The ideas presented here are the first steps toward the implementation of a mechanistic model for core disassembly. Some of the previous work available from public sources related to the thermal deformations of the fuel channels in pressurised heavy water reactors (PHWR), under different circunstances covered within the analysis of both design basis accidents and beyond design basis accidents (e.g. LOCA/LOECCS, loss of all heat sinks), include the description of the ballooning deformation of the pressure tube (PT) into contact with the calandria tube (CT) in a CANDU reactor using a dynamic lumped parameter model, and assuming conservative limits in accordance with existing experimental data, providing the means to construct a fuel channel integrity map defining zones in the parameter space where sufficient conditions are provided to ensure the integrity of the fuel channel [3]. Another example is the study case of the sagging and balloning deformations in the context of a stagnation channel break in an Indian PHWR [4], computer simulations were used to generate a map to predict the conditions (pressure and temperature) for the occurrence of the contact between the PT and the CT. More recently Atomic Energy Canada Limited (AECL) initiated a severe accident analysis program using the MAAP-CANDU computer code to support level 2 probabilistic safety assessment (PSA). The deformations of a single scaled-down fuel channel in a severe accident situation was studied from the experimental point of view [5]. The objective of the study was to fill the lack of data for MAAP-CANDU code in the case of severe core damage accident. Computer simulations were implemented and validated againts the experimental data, the details were presented in [6]. The results obtained in this program were included in the development process of the severe accident management guidance (SAMG) for the Canadian nuclear industry [7].

Currently the general progression of a severe accident in CANDU reactors is fairly well understood [1, 2]. During the initial stages of the accidents high-temperature transients are developed at rates that strongly depend on the specific state and geometrical configuration of the reactor at the initial time (power distribution, temperatures, pressures, etc) and material properties. These high-temperatures weaken the PT causing ballooning and sagging. As the accident

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progress in time the PT will contact the CT creating a path to transfer heat from the fuel to the heavy water (moderator) surrounding the fuel channel. If the moderator cooling system is not available this heat transfer could lead to the boiling of the moderator and even lead to a configuration where some of the fuel channels will be completely exposed. Continuous increase in the temperature of the system could lead to a complete deformation (sagging) of the PT/CT system and structural failure or cracks could develop on the supportive structure of the fuel channels causing the collapse of the uncovered channels onto the submerged ones. This process will eventualy lead to the disassembly of the reactor core. A clear understanding of the main physical phenomena involved in this type of events is essential to produce simulations that, when compared with available experimental data, could give us a realistic estimate of the timing and stages of the process evolution as well as the needed criteria based on the involved variables that allow us to implement management procedures for this kind of beyond design basis accidents.

The organization of the paper is the following, in the next section a the available experimental/computational results related with the core disassembly arereviewed and summarized. This approach will help us to identify potential improvements to the currently used mathematical models. Section III is devoted to the compilation of the main physical properties of the materials relevant for the analysis. In the last section some of the ideas of possible directions of development toward a complete core disassembly computational code are presented.

II. CORE DISASSEMBLY: EXPERIMENTAL AND COMPUTATIONAL RESULTS

Luxat [1] presented a very detailed analysis of the progression to severe accident in a CANDU reactor from the thermalhydraulic point of view clearly identifying the physical conditions of the core at the onset of the reactor heat-up: the HTS will be completely voided, the intact PT will be in contact to the CT in the fuel channels (ballooning deformation), the HTS and the calandria vessel (CV) will be at sub-atmospheric pressure due to the opening of one or more of the four CV rupture disks allowing depressurization of the CV through discharge to the containment, the moderator will be partially boiled-off and from 6 to 10 fuel channel rows will be uncovered, the fuel in the intact fuel channels is expected to be at a temperature $T \sim 300^{\circ}C$ and generating decay heat at the level of $0.8\% FP$, the shield tank (ST) is expected to be full with light water and subcool ($T < 80^{\circ}C$). The subsequent mechanical, thermal and chemical interactions between the fuel channels and the remaining two-phase moderator inside the CV will rules the core disassembly process.

Series of experiments simulating the previously described initial conditions were conducted in the Core Disassembly Test Facility (AECL Whiteshell Laboratories) [5]. The goal of the experiments was to understand the mechanical deformations that a single fuel channel undergoes under severe accident conditions, the effects of the mechanical and thermal interaction between channels as well as the chemical interactions with the surrounding were not considered. During the tests different parameters were measured: temperature at the top and the bottom of the channel at different positions, channel end-load, sag at channel's mid-point, channel longitudinal displacement, and channel power. Post-test procedures included the measuring of the final sag profile, changes on the original diameter of the PT, top and bottom wall thickness along the channel, final position of the heaters and estimation of the localized axial strain along the bottom side of the channels. The main results of this study can be summarized as: no significant sag was observed for $T_{bottom} < 800^{\circ}C$, the magnitude of the sag at the mid point of the channel is directly related to the heated length and heat-up rate, the temperature at the bottom of the channel near to the mid point is always about $200^{\circ}C$ higher than at the top, in almost all the cases the measured sag deformation is large enough that the channel will touch the next one underneath, the load recorded at the free end of the channel were no sufficient to pull-out the channel neither during the deformation period nor during the cooldown, large wall thinning was observed in the bottom of the channel one or two bundles away from the mid point, and about one bundle away of both ends of the channel on the top side (the wall thinning was concentrated in the space between bundles), the cross section of the channel became oval at the regions of higher temperatures, the maximum of the axial localized strain at the bottom of the channel was situated in the gap between the bundles one or two bundles away from the channel mid point (in coincidence with the localization of the wall thinning region). From these results the authors derived the following conclusions:

- strong indication that time-dependent creep deformation is the leading mechanism for sagging,
- based on the localization of the wall thinning along with the maximum strain it is expected that the PT and CT debris formed due to core disassembly will be two to three bundles long,
- during the first stages of the sagging process it is possible to inject coolant into the channel as part of the severe accident management actions without failing the channel.

Computer simulations were implemented and validated againts the experiments in order to capture the main physical processes related with the sag deformation of the fuel channels [6]. Two different models were implemented:

time-dependent inelastic deformations caused by yielding of the material and time-dependent creep deformations. Although both models predicted a similar pattern on the sag behaviour the code based on the creep deformations seemed to be more accurated but more expensive from the computational point of view and therefore discarted. More in details the first model was based on a finite element implementation of a two-dimensional beam elements model with a circular cross section, a nonuniform nodal grid was used in the calculation to ensure the correct description of the strain-stress in the channel. Appropriate boundary conditions were imposed (one end fixed and the other coupled to a variable stiffness spring) and the assumed temperature distribution around the circunference of the channel was input to the code. The material properties used in the implementation were the following: the temperature dependent modulus of elasticity, the coefficient of thermal expansion, and the empirical strain creep rates in the longitudinal direction (some of the used properties were for Zircaloy-4 instead of $Zr-2.5\%Nb$). The code was calibrated/validated against experiments leading to very good agreement with the measured sag profile (within 2%). It is needed to call our attention to the fact that despite of the careful selection of the material properties and the emphasis on the special treatment of the nodal grid included in the calculation still an "acceleration factor" should be introduced in the longitudinal creep rate in order to obtain quantitative agreement with the experimental data. This might be an indication that either some physical processes are not included in the simulation or new material properties are needed. In the next section the main material properties used in the simulation are reviewed and in the final section ideas of how to improve the physical model are presented.

III. MATERIAL PROPERTIES REVIEW

In the analysis/simulation of thermal deformations of alloys special attention should be devoted to several materials properties like the thermal conductivity, Young's modulus, Poisson ratio, yield stress, ultimate stress, fracture strain and creep rates, and coefficient of thermal expansion. The information available from public sources regarding these properties are scattered and sometimes very incomplete. The following is a review of some of these properties from public sources.

In CANDU reactors different grades of Zirconium alloys are used for the PT and the CT. The PT are made of a corrosion resistant binary Zirconium/Niobium alloy $Zr-2.5\%Nb$ and the CT uses Zircaloy-2 with a nominal composition $Zr-1.5\%Sn-0.15\%Fe-0.1\%Cr-0.05\%Ni$.

The Zirconium alloys have some properties very similar to the elemental Zirconium, both have two crystallographic phases α and β. The change from one phase to the other happens with the increase of temperature, in the case of the pure Zirconium the allotropic form is α for temperatures less than $865^{\circ}C$ with a crystal structure *hcp* (anisotropic), and β for higher temperatures with crystal structure *bcc* [8] (isotropic). In the case of the alloys the transformation from one phase to the other happen within an interval of temperatures, for example for Zircaloy-2 and Zircaloy-4 alloys the transformation from α to $\alpha+\beta$ phase happens at $\sim 810^{\circ}C$ and from $\alpha+\beta$ to β at $\sim 980^{\circ}C$ [9].

Correlations for the transversal creep strain rates were obtained by Shewfelt *et al* [10] based on constant-stress uniaxial tests (hoop stress) for the $Zr-2.5\%Nb$ alloy, the tests were run at constant temperatures. It was found that in the tested material the allotropic transformations $\alpha/(\alpha+\beta)$ and $(\alpha+\beta)/\beta$ happened at temperatures of $610^{\circ}C$ and $925^{\circ}C$ respectively. The results of the creep tests showed that for temperatures in the range $450^{\circ}C-700^{\circ}C$ the creep curve shows a very short primary creep region followed by a large secondary region, between $750^{\circ}C$ and $900^{\circ}C$ the creep curves show a large primary region, and in the temperature range $950^{\circ}C-1200^{\circ}C$ a small inverted primary creep region was observed followed by a large secondary region. Plots of creep rates vs. applied stress at different temperatures showed that in the range of temperatures $450^{\circ}C-500^{\circ}C$ the stress exponent was constant (~ 9) over the stress range used, for temperatures between $700^{\circ}C$ and $850^{\circ}C$ the stress exponents varied between 1.4 and 1.8, and for temperatures in the range $950^{\circ}C-1200^{\circ}C$ constant stress exponent in the order of 3.4 was observed. This behavior led the authors to consider two main deformation mechanisms: power law creep at the α phase ($450^{\circ}C<T<500^{\circ}C$) and in the β phase ($T>950^{\circ}C$), and grain-boundary sliding during the transition phase ($550^{\circ}C<T<850^{\circ}C$). Based on the experimental data and by combining the identified deformation mechanisms with different nature hardening processes happening during the allotropic transformations two creep strain rates were proposed

$$\dot{\epsilon}(\sigma,T,t)=\begin{cases}1.3\times10^{-5}\sigma^{9}\,t\,e^{-36600/T}+\dfrac{5.7\times10^{7}\sigma^{1.8}e^{-29900/T}}{\left[1+2\times10^{10}\int_{t_1}^{t}e^{-29900/T(\tau)}\,d\tau\right]^{0.42}}, & 450^{\circ}C<T\leq850^{\circ}C\\ 10.4\,\sigma^{3.4}\,t\,e^{-19600/T}+\dfrac{3.5\times10^{4}\sigma^{1.4}e^{-19600/T}}{1+274\int_{t_2}^{t}e^{-19600/T(\tau)}[T(\tau)-1105]^{3.72}\,d\tau}, & 850^{\circ}C<T<1200^{\circ}C\end{cases}\tag{1}$$

where the units for the creep strain rates are s^{-1}, the stress is given in MPa, and the temperatures T are in K.

Temperature ($^{\circ}C$)	K_2 (MPa^{-1})
800	0.0119
825	0.0114
850	0.0167
875	0.0134
900	0.0100

TABLE I: Values of the temperature dependent constant K_2 in equation (2)

Additionally t_1 is the time when $T = 700^{\circ}C$ and t_2 when $T = 850^{\circ}C$. The presented correlations were tested against experiments (uniaxial and biaxial creep test) with values of stresses in the range $3MPa < \sigma < 100MPa$ and ramps of temperatures between $1^{\circ}C/s$ and $50^{\circ}C/s$.

Using four-point bend tests correlations were proposed for the longitudinal creep strain rates for the $Zr - 2.5\%Nb$ alloy [11]. The tests consisted in increasing the temperature of the sample at a constant rate (less than $5^{\circ}C/s$) up to the test temperature under full load and then measuring the time dependence of the strain at that temperature. Tests were run at different temperatures in the interval $800^{\circ}C < T < 950^{\circ}C$ for stresses between $0.4MPa$ and $1.2MPa$. Very small creep rate was observed for $T < 750^{\circ}C$. The lower the applied stress was the larger the secondary region was in the creep curve with a decrease in the slope as the stress decreased. By taking the ratio strain/stress for different temperatures and stresses as a function of time the authors showed that there was a linear relationship between the strain and the stress within the measured range of temperatures and stresses. Another interesting observation was that for a constant stress the variation of the strain curve with temperature showed first and increase reaching the maximum at $T = 850^{\circ}C$ and then decreasing, the strain curve is almost constant for $T = 950^{\circ}C$, featuring a departure from the normal behavior of the creep curves [12]. The authors related the linear variation of the strain as a function of the applied stress with previously published work where this behavior was observed in pure Zirconium when small stress was applied at temperatures near the phase transition temperature due basically to internal stresses produced by volume changes. From this analysis the following creep strain rate was proposed

$$\dot{\epsilon}(\sigma, T, t) = 8 \times 10^{10} \sigma \, e^{26670/T} \left(K_2 - \epsilon/\sigma\right)^{2.4}, \;\; 800^{\circ}C \leq T \leq 900^{\circ}C \tag{2}$$

where the units are s^{-1} for the creep strain rate, MPa for the stress, and K for the temperature. The values of the temperature-dependent constant K_2 are given in Table I. For $T < 750^{\circ}C$ $K_2 = 0$, in the range $750^{\circ}C < T < 800^{\circ}C$ the value of the constant is $K_2 = 0.0119\, MPa^{-1}$, for $900^{\circ}C < T < 950^{\circ}C$ $K_2 = 0.01\, MPa^{-1}$, and for $T > 950^{\circ}C$ the strain rate was zero. There was a relative good agreement between the proposed correlations and the experimental data for different ramps in temperature.

Thermal conductivity correlations for $Zr - 2.5\%Nb$ are included in the Material Properties Database from the International Nuclear Safety Center (INSC) [14] based on the compilation of data from different experiments using speciments with different heat treatments. In the α phase ($500K - 1100K$) the best fit to the available data in the axial direction is given by the equation

$$k(T) = 16.85 - 2.186 \times 10^{-3} T + 8.899 \times 10^{-6} T^2 \tag{3}$$

where the units for k are $Wm^{-1}K^{-1}$ and the temperature is in K. The uncertainty in the values given by this correlation is of 5%. An interesting fact is that the available data for the thermal conductivity in the circular direction within the α phase for cold-worked as well as for heat-treated speciments are well discribed by this correlation (the α phase has an anisotropic atomic structure). No information is included regarding to the measurement of the texture of the tested speciments. The correlation in the β phase ($1130K - 1600K$) is given by the expression

$$k(T) = 5.0 + 0.020T \tag{4}$$

the units are the same as for the correlation in the α phase and the uncertainty is of 15%. There is no data presented within the transition region between the α and the β phases.

A detailed review of the extensive amount of experimental data related with thermal conductivity of Zircaloy-2 and Zircaloy-4 is included in the database from INSC [15], the statistical analysis of the presented data led to the following recommended correlation for the thermal conductivity of Zircaloy

$$k(T) = 12.767 - 5.4348 \times 10^{-4} T + 8.9818 \times 10^{-6} T^2 \tag{5}$$

where the units are the same as for the correlations in the $Zr - 2.5\%Nb$ case. The uncertainties of this correlation increase from 4% at $300K$ to 7% for higher temperatures ($T > 1200K$). Contrary to the case of the $Zr - 2.5\%Nb$

alloy, only one expression is provided independently of the temperature (allotropic phase), and alloy composition (Zircaloy-2 or Zircaloy-4).

Regarding to the thermal expansion coefficient, the database from INSC contains a review where new correlations (different from those recommended in MATPRO [16]) are included. Again the correlations were obtained from the analysis of the existing experimental data for Zircaloy-2, Zircaloy-4 and elemental Zirconium, and even for these materials the amount of data available measuring the thermal expansion in different directions is very incomplete. The recomended correlations are the following: for the α phase ($300K < T < 1083K$)

$$\left(\frac{\Delta L}{L}\right)_{radial} = -2.128 \times 10^{-3} + 7.092 \times 10^{-6} T \tag{6}$$

$$\left(\frac{\Delta L}{L}\right)_{axial} = -1.623 \times 10^{-3} + 5.458 \times 10^{-6} T \tag{7}$$

$$\left(\frac{\Delta L}{L}\right)_{circum} = -2.998 \times 10^{-3} + 9.999 \times 10^{-6} T \tag{8}$$

where the temperature is measured in K. For the transition region only one correlation is presented

$$\left(\frac{\Delta L}{L}\right)_{axial} = -6.528 \times 10^{-3} + 9.796 \times 10^{-6} T + 6.187 \times 10^{-4} e^{\frac{(T-1063)^2}{2130}} \tag{9}$$

In the β phase ($T > 1144K$) also one correlation is presented

$$\left(\frac{\Delta L}{L}\right)_{axial} = -6.394 \times 10^{-3} + 9.7 \times 10^{-6} T \tag{10}$$

The uncertainties in the α phase for the radial and axial directions when compared with the experimental data are of 15% and 12% respectively, and in the case of the β phase the uncertainty is 20%. These correlations are recommended in the cases where no information about the texture of the material is available, when information is available about the texture of the material then the single crystal correlations from MATPRO [13] are recommended. Special attention should be devoted to the oxygen content of the analyzed material as well as to its heat treatment.

The Young's modulus as a function of the temperature is given by the relationship [4]

$$E(T) = \begin{cases} 1.088 \times 10^{10} - 5.475 \times 10^{7} T, & T < 1090\,K \\ 4.912 \times 10^{10} - 4.827 \times 10^{7} (T - 1090), & 1090\,K \leq T \leq 1240\,K \\ max(10^{10}, 9.21 \times 10^{10} - 4.05 \times 10^{7} T), & T > 1240\,K \end{cases} \tag{11}$$

No units are presented, and there is no mention to what material this correspond to.

IV. IMPROVING THE PHYSICAL MODEL

The computer simulations regarding the deformations of a single fuel channel [6] seem to capture the qualitative side of the transient process, but only after the introduction of a fictitious "acceleration factor" the experimentally detected amount of sagging can be reproduced. Beside this the presented results were validated only againts one set of experimental data, raising the question whether after its introduction is the same "acceleration factor" able to reproduce all the experimental results quantitatively. Despite the results of the model and the need for improvements it is our opinion that the problem of the behavior of a single channel during severe accident conditions is solved.

The future work related with the subject of core disassembly in CANDU reactors should focus on the experimental/computational study of the interaction between fuel channels during the severe accident conditions. Although there is some evidences about experimental work in this area no result have been reported in the public literature, and no simulations, to the best of our knowledge, have been done in this area neither. Several problems can be mentioned that need to be assessed in future studies in the area of core disassembly:

- Where inside the core the disassembly process will start, this question is directly linked to the status of the core when the reactor trip happened due to the fact that the decay heat level at each channel is linked to the channel power during operation. The sag deformation of the fuel channels is a temperature driven process and therefore directly linked with the levels of decay heat.

- Once a fuel channel deforms into contact to the next channel underneath, the load distribution of the lower channel will change as well as its temperature distribution in the axial and in the circumferential directions. The effect of these changes will affect the dynamics of the deformation process of the lower channel.

- As the uncovered channels sag wall thinning happen in the regions between the bundles. It is possible that even before the channel fails some crack will be developed on the calandria tube opening a path to steam to areas where good conditions exist to increase the reaction rate with the Zircaloy material, leading to changes on temperature and increasing the hydrogen production.

- The failure process of the channels is expected to be depending on its position whether it is a submerged or an uncovered channel. In the case of submerged channels, those are expected to deform due to the increase on the bending load due to the accumulation of debris from upper channels upto the moment when the rolled joint of the PT/CT fail and the channel collapses. In the case of the uncovered channels their rupture failure will be due to the wall thinning process.

Advances in any of these directions will greatly increase our understanding of the core disassembly process in a CANDU reactor. From the computational point of view accurate mechanistic models can be developed for the analysis of each one of the previously mentioned problems with heavy dependences on material properties and computational resources, or more "toy-model" type description can be adopted where along with the implementation of some of the currently used failure criteria could lead to and improved estimate of the timming of the whole process.

At this moment we consider that based on the previously presented review on material properties showing the incompleteness of the experimental data, it seems that the "toy-model" description will be favored.

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