COUPLING RELAP5 AND PRESSURE TUBE DEFORMATION MODELS TO ANALYZE THE THERMAL-MECHANICAL PHENOMENA IN CANDU SEVERE ACCIDENTS

F. Zhou[1], D.R. Novog[1], L. J. Siefken[2], C. M. Allison[2]
[1] McMaster University, Hamilton, Ontario, Canada
[2] Innovative System Software, Ammon, Idaho, USA
zhouf5@mcmaster.ca, novog@mcmaster.ca
mlmsiefken@gmail.com, iss@cableone.net

Abstract

During the channel heat-up phase of postulated severe accidents in CANDU reactors,the pressure tube may balloon or sag into contact with its calandria tube depending on the internal pressure. If the channel is surrounded by the moderator, this contact will establish an effective heat sinkto the moderator.If the channel is uncovered, the fuel channel assemblywill sag or disassemble. These phenomena, which have significant effects on accident progression, however, are not mechanisticallymodeled by most existing severe accident codes. Three channel deformation modelsbased on existing phenomena in literature have been coupled toRELAP5 to provide more robust treatment of the deformation phases of severe accidents. Two coupling methods are used: one usesa Python script to externally couple these models withRELAP5/Mod3.3;in the othermethod,the models are compiledintoRELAP/SCDAPSIM/Mod3.6 as newSCDAP subroutines. The main objectives of this paper areto introduce these models and the coupling methods, and to benchmarkthemagainst several PT deformation experiments.

Nomenclature

α, β	accommodation parameter and fluid parameters
ε_{pt}	creep strain
ε_f	pressure tube failure strain
$\dot{\varepsilon}_{pt}, \dot{\varepsilon}_{ct}, \dot{\varepsilon}_{\alpha}$	creep strain rate, s^{-1}
σ_{pt}, σ_{ct}	stress, MPa
σ, σ_0	surface roughness, μm
Λ	mean free path, μm
c	distance to the centroid of the cross-section, m
c_1	Vickerscorrelation coefficient, GPa
c_2	Vickers size index
d	maximum possible depth of local defect, μm
E	Young's modulus, $\mathrm{N/m^2}$
f_g	correction term
h	conductance, W/m^2K
H_c	contact micro-hardness, GPa
I	Moment of inertia, m^4
k_g, k_s	thermal conductivity, W/mK
K_{pl}, K_{el}	plastic and elastic curvature, m^{-1}
m	mean surface asperity slope
M	bending moment, $\mathrm{N \cdot m}$
n	creep stress exponent
P_c	contact pressure, GPa
t	time, second (s)
T	temperature, kelvin (K)
w_0	initial wall thickness, μm
x	axial distance, m
y	deflection in the vertical direction, m
Y	mean plane separation, μm

1. Introduction

The CANDU fuel channel consists of a Zr-2.5wt.%Nb Pressure Tube (PT) containing 12 (or 13) fuel bundles. The PT is surrounded by the Zircaloy-2 Calandria Tube (CT) which is contained in a large calandria vesselfilled with heavy water acting as moderator. The two CT ends are rolled into the lattice tube ends at the inner tube sheets, while the PT are connected to the end fittings at two ends by rolled joints. The annulus between the PT and the CT is filled with CO_2 to reduce heat loss to the moderator. Four garter springs are put into the annulus to support the PT and prevent PT/CT contact during normal operation.Under accident conditions where channel heatup cannot be precluded, the fuel channel may undergo a variety of deformations since the range of accident conditions (pressures, temperatures, liquid stratification, and moderator liquid environment) may be diverse and dependent on system and operator responses.

If the internal pressure is high (>1MPa), the dominant PT deformation mechanism is ballooning, i.e. the PT expands radially towards the CT. Ballooning is a result of transverse creep strain under large hoop stresses when the PT experiencing temperature ramps. If the circumferential temperature distribution of the PT is relatively uniform, the PT will balloon into contact with its CT establishing an effective heat path to the moderator. However, if the coolant in the channel is stratified, the PT is very likely to experience non-uniform temperature distribution which leads to non-uniform transverse creep strain. Such non-uniform heat-up and strain may or may not fail the fuel channel depending on a number of factors.

A number of models have been developedby other researchers to model the ballooning of PTs. Most of them use the creep strain rate equation for Zr-2.5wt%Nb developed by Shewfelt et al.[1]. The TRAN II code assumes that the PT circumferential temperature is uniform, and uses only the average temperature of PT to predict transverse strain[2].For non-uniform PT-ballooning models, the PT circumference is divided into sectors, and the strain of each sector is calculated independently based on its local temperature and stress. It is often assumed that the PT remains circular during ballooning, e.g. GRAD [3] and NUBALL [4]. Although these circular models precluded the possibility of local PT/CT contact, they are found to predict the ballooning of PT in experiments reasonable well. An improved model to predict non-circular PT deformation has been developed by Lei et al. [5], aiming to improveaccuracy when circumferential temperature gradientsare large and the model allows the hottest area of the PT to deform intocontact with the CT first. In most ofthese models, the same failure criteria are used, i.e. the PT is assumed to fail due to local necking. A lower and upper bound of the failure criteria are available[6]: the upper bound criterion assumes that the PT thickness is uniform and failure occurs when the tube necks down to zero wall thickness; the lower bound criterion assumes that there are defects on the PT and the defects happen to coincide with the local hot spot which causes the tube to neck down to zero more quickly. If the average circumferential strain of the PT exceeds ~18% (the amount of strain required for PT to balloon and fully contact the CT) before the local strain at a hot spot reaches the failure limit, the PT failure is prevented provided that its CT is sufficiently cooled.

If the ballooning contact is made, a large heat flux spike into the moderator is expected since the PT is at very high temperatures. This heat flux spike may cause film boiling on the CT outer surface. Experiments have shown that in most cases thesefilm boiling patches will be cooled and rewet due to heat transfer to and from surrounding regions of nucleate boiling [7]. For cases at low moderator subcoolings and high heat fluxes, rewetting may be prevented which may causeboth the PT and the CT to strain and fail.

Luxat [8] developed a lumped parameter model to study the heat transfer process during PT-CT ballooning contact. It was concluded that the PT contact temperature, contact conductance and moderator subcooling are three important parameters that influence CT dryout phenomena. The rapid drop in contact conductance is due to the changes in the thermal-expansion of two tubes during the temperature transient. It was also found that using the minimum film boiling temperature method, the measured duration of dryout time was well predicted and that the film boiling behavior is governed by the post-contact heat transfer to the PT rather than the PT temperature at contact. Cziraky [9] presented in his thesis a new approach to calculate the contact conductance during PT-CT ballooning contact. The contact pressure was iteratively solved by equating the creep strain rate equations of the PT and the CT. A modern correlation developed by Yovanovich et al. [10] was then used to calculate the contact conductance for both initial-contact and post-contact phases. This approach predictedvery high contact conductance at initial contact followed by a rapid decrease in conductance which is consistent with experimental findings. The model was used to predict two contact boiling experiments [11][12]. The predicted peak contact conductance differs by a maximum of 5% and equilibrium valuesby a maximum factor of 2.0[9].

When the internal pressure is low (<1MPa), the dominant deformation mechanism is PT sagging.Sagging occurs during $\alpha + \beta \rightarrow \beta$ phase transformation, thus the temperature at which the deflection becomes noticeable is higher than that associated with ballooning phenomena. As the PT sags downwards it will contact its CT. The contact pressure and contact area are much smaller compared to ballooning contact. In the short term, this sagging contact is less of a concern as it is not likely to cause extensive film boiling on the CT outer surface.PT-CT ballooning/sagging contact lowers the maximum core temperature and delays channel failures. Meanwhile,the heat deposited into the moderator also increases and the moderator may undergo boiling. As the moderator level drops, channels at the higher elevationsin the calandria are uncovered. The uncovered channel will then quickly heat-up, sag and contact the lower channel.As sagging increases, the fuel channel may separate at its bundle junctions transferring both heat and loads to the lower channels.

When simulating a postulated severe accident many existing computational tools utilize simple user-input threshold temperatures to determinePT-CT contact, channel failure and disassembly, e.g., in MAAP-CANDU[13], ISAAC [14]and SCDAP/RELAP5 [15]. While such threshold models are simple and easy to integrate in larger computer programs, since they lack models based on physical deformation processes, and hence cannot aid in our understanding of the sensitivity and uncertainty in the accident predictions.Toquantitatively study the impact of these phenomena on accident progression, three mechanistic models which can be coupled with system code RELAP5 have been developed:

- “BALLOON” calculates the transverse strain of PT/CT and the contact conductance after ballooning contact;
- “SAGPT” calculates the longitudinal strain and the deflection of PT and determines the PT-CT sagging contact;

- "SAGCH" models the sagging of afuel channel assembly after uncovery, determines channel-to-channel contact, and calculates CT-CT contact heat transfer.

Two different coupling methods are used which transfer the local thermalhydraulic conditions from RELAP to the mechanistic models. The first one uses a Python script to externally couple these models with RELAP5/Mod3.3 in which the PT-annulus-CT structure is represented by a normal heat structure. In the second method, these models are compiled into RELAP/SCDAPSIM/Mod3.6 as new SCDAP subroutines, and the PT-annulus-CT is represented by the SCDAP shroud component which gains additional capabilities to model 2D conduction and various severe accident phenomena. The main purposes of this paper are to introduce these models and the two coupling methods, and to benchmarkthem against several PT deformation experiments.

2. Model description

2.1Model for PT Ballooning–"BALLOON"

The PT ballooning model is based on reference [9] with the severalimprovements. In reference [9], the creep strain rate was calculated with only the numerator of the grain boundary term which covers a relatively small temperature range. In "BALLOON", the complete set of creep strain rate equations by Shewfelt et al.[1] are used covering a temperature range from 450^{o}C up to 1200^{o}C.The computer algorithmto find the contact pressure between PT and CT are also improved to allow fast convergenceduring the transient.

The circumferential temperature of PT is assumed to be uniform because neither the RELAP5 heat structures (1D, radial) nor SCDAP core components (2D, radial & axial) are solving conduction equations in the circumferential direction. The transverse strain is calculated independently at each axial location of a channel. The thin-wall assumption is used when calculating the hoop stresses of the pipessince the thicknesses of the PT and the CT are relatively small compared to their diameters.

2.1.1 PT creep strain rate equation

For temperature below 450^{o}C, the creep strain rate of PT is assumed to be zero. For temperature between 450^{o}C and 850^{o}C, the creep deformation of PT is due to two mechanisms, i.e. power law creep in α-phase and grain boundary sliding[1]. Thusthe creep rate is the sum of two terms:

$$\dot{\varepsilon}_{pt} = \dot{\varepsilon}_{\alpha} + \dot{\varepsilon}_{gb} = 1.3 \times 10^{-5} \sigma_{pt}^{9} \exp\left(-\frac{36600}{T}\right) + \frac{5.7\times10^{7}\sigma_{pt}^{1.8}\exp\left(-\frac{29200}{T}\right)}{\left[1+2\times10^{10}\int_{t1}^{t}\exp\left(-29200/T\right)dt\right]^{0.42}} \quad (1)$$

$t_1$is the time when$T$ = 700^{o}C, the denominator of $\dot{\varepsilon}_{gb}$is to account for the hardening due to grain growth for temperature above 700^{o}C.For temperature between 850^{o}C and 1200^{o}C, the creep rate equation of the PT is again the sum of two terms[1]:

$$\dot{\varepsilon}_{pt} = \dot{\varepsilon}_{\beta} + \dot{\varepsilon}_{gb} = 10.4\sigma_{pt}^{3.4} \exp\left(-\frac{19600}{T}\right) + \frac{3.5\times10^{4}\sigma_{pt}^{1.4}\exp\left(-\frac{19600}{T}\right)}{1+274\int_{t2}^{t}\exp\left(-\frac{19600}{T}\right)(T-1105)^{3.72}dt} \quad (2)$$

in which $\dot{\varepsilon}_\beta$ is due to power law creep in β-phase and $\dot{\varepsilon}_{gb}$ is due to grain boundary sliding.The denominator of $\dot{\varepsilon}_{gb}$ is to account for the hardening caused by rapid phase transformation above 850°C, and t_2 is the time when T = 850°C.$\dot{\varepsilon}_{gb}$ decreases rapidly, thus for temperature above 950°C, this term becomesnegligible. Unless otherwise noted, T in all the equations of this paper is in the unit of kelvin (K).

2.1.2 CT creep strain rate equation

The transverse creep rate equation of CT for temperature below 850°C is the sum of the dislocation creep term and the grain boundary sliding term[16]:

$$\dot{\varepsilon}_{ct} = \dot{\varepsilon}_d + \dot{\varepsilon}_{gb} \qquad (3)$$

$$\dot{\varepsilon}_d = 22000(\sigma_{ct} - \sigma_i)^{5.1}\exp(-34500/T_{ct}) \qquad (4)$$

$$\sigma_i(t) = 1.4 + \int_0^t [110\dot{\varepsilon}_d - 3.5 \times 10^{10}\sigma_i^{1.8}\exp(-34500/T_{ct})]dt \qquad (5)$$

$$\dot{\varepsilon}_{gb} = 140\sigma_{ct}^{1.3}\exp(-19000/T_{ct}) \qquad (6)$$

Following the PT/CT contact, it is assumed that the creep strain rate of PT equals to that of the CT, i.e. $\dot{\varepsilon}_{pt} = \dot{\varepsilon}_{ct}$. The contact pressure P_c between PT and CT is then iteratively calculated.

2.1.3 Contact Conductance

When PT/CT contact is made, the contact conductance is calculated using model developed by Yovanovich et al. [10]. In Yovanovich's model, the interfacial conductance is the sum of two components, i.e.

$$h = h_c + h_g \qquad (7)$$

h_c is due to metal-to-metal contact and h_g is the conductance across the gas gap. They can be calculated using the following correlations:

$$h_c = 1.25\frac{k_s m}{\sigma}\left(\frac{P_c}{H_c}\right)^{0.95} \qquad (8)$$

$$h_g = \frac{k_g f_g}{Y + \alpha\beta\Lambda} \qquad (9)$$

In which P_c is the contact pressure, m is mean surface asperity slope, σ is the surface roughness,H_c is the contact microhardness, Y is the mean plane separation, and $\alpha, \beta, \Lambda, f_g$ are the correction terms. H_c can be explicitly calculated:

$$\frac{P_c}{H_c} = \left[\frac{P_c}{1.62c_1(\sigma/\sigma_0 m)^{c_2}}\right]^{1/(1+0.071c_2)} \qquad (10)$$

In which c_1, c_2 are the Vickers correlation coefficient and Vickers size index. Y is approximated using the following correlation:

$$\frac{Y}{\sigma} = 1.184\left[-\ln(3.132\frac{P_c}{H_c})\right]^{0.547} \qquad (11)$$

2.1.4 Failure Criteria

The failure criterion in reference [17] was validated for a wide range of experimental conditions: the PT is assumed to fail when the local transverse strain at any point exceeds

$$\varepsilon_f = -\frac{1}{n}\ln\left[1-\left(\frac{w_0-d}{w_0}\right)^n\right] \qquad (12)$$

where w_0 is the initial wall thickness, *d* is the maximum possible depth of a local defect, and *n* is the creep stress exponent. While equation (12) is a local failure criterion, BALLOON is a one dimension model and calculates only the average creep strain. Experiments have shown that for moderate circumferential temperature variation (30°C to 70°C) the specimens normally did not fail until the average creep strain of 20% was reached, i.e. after the PT has ballooned into contact with CTs; for tests with more severe circumferential temperature distribution (>100°C), the specimens all failed at an average creep strain of less than 20%[3]. The model currently uses a user-input failure criterion and its value is normally set to 20%.

2.2Model for PT Sagging–"SAGPT"

2.2.1 Basic Theory

Sagging of the PT is caused by longitudinalbending stress. The loads causing it to sag are its self-weight, weight of coolant and the weight of fuel bundles. Besides the supports at the two ends atthe lattice tube bearing, the PT is also supported by the four garter springs. "SAGPT" is only called when the CT temperature is sufficiently low that the CT will not sag due to creep strain; otherwise, the channel sagging model (SAGCH) described in section 2.3 will be called. To simplify the model, the four garter springs are assumed to be rigid, i.e. they will not move or deform. Simple beam theory is used, and the PT is assumed to have two fixed ends at its two rolled joints. The deflection of the PT is the sum of elastic and plastic bending. The curvature of the beam due to elastic strain is

$$K_{el}(x,t) = \frac{M(x,t)}{E(x,t)I(x)} \qquad (13)$$

$M(x,t)$ is the bending moment at *x*. $I(x)$ is the moment of inertia of the pipe,and $E(x,t)$ is the Young's modulus which is a function of temperature. The longitudinal stress across a section at location *x* where the bending moment is *M*(*x*) can be expressed as follows:

$$\sigma(x,t) = -\frac{M(x,t)c}{I(x)} \qquad (14)$$

where c is the distance to the centroid of the cross-section. With the above stress, the longitudinal creep strain can be calculated by integrating the creep strain rate equation. The curvature of the beam due to plastic strain is

$$K_{pl}(x,t) = -\frac{\varepsilon(x,t)}{c} = -\frac{\int_0^t \dot{\varepsilon}(x,t)dt}{c} \qquad (15)$$

The total curvature is then the sum of elastic curvature and plastic curvature, i.e.

$$K_t(x,t) = K_{el}(x,t) + K_{pl}(x,t) = \frac{\frac{d^2y}{dx^2}}{\left[1+\left(\frac{dy}{dx}\right)^2\right]^{3/2}} \approx \frac{d^2y}{dx^2} \qquad (16)$$

Deflection *y* can be calculated by integrating twice the curvatures along *x*.

2.2.2 Longitudinal strain rate equation

Sagging will only occur during $\alpha + \beta \rightarrow \beta$ phase transformation since the stress due to bending is insufficient to sustain plastic flow on its own. The internal stress caused by phase transformation together with the stress due to bending produces longitudinal strain. The longitudinal strain rate equation used in the model is developed by Shewfelt et al. [18]. It can be expressed as follows:

$$\dot{\varepsilon} = 8 \times 10^{10} \sigma \exp\left(-\frac{26670}{T}\right)\left(K_2 - \frac{\varepsilon}{\sigma}\right)^{2.4} \qquad (17)$$

K_2 is a function of temperature given by table 1.

Table 1 Constant K_2 in the longitudinal creep strain rate equation

Temperature (^oC)	K_2 (MPa^{-1})
T<700	0.0
700<T<800	0.0119
800	0.0119
825	0.0114
850	0.0167
875	0.0134
900	0.0100
900<T<950	0.0100
T>950	0.0

Between 800^{o}C and 900^{o}C, K_2 is obtained by linear interpolation between two the adjacent values. This creep strain rate equation is based on data from constant-temperature and constant-stress experiments. During the sagging of the PT (or CT), both the temperatures and stresses change with time. Validation tests have been carried out by Shewfelt et al. [18] to validate the equation during a temperature transient. In these tests, the PT specimens were heated up at different rates under constant stress. The data were compared to that predicted by the creep strain rate equation, and excellent agreements were observed. However, if the stresses are not constant, the equation must be modified. The $\frac{\varepsilon}{\sigma}$ in the bracket is used to estimate the current volume fraction of β-phase at a given time. According to De Jong et al. [19] the strain caused by a phase transformation under constant stress varied linearly with the amount of material transformed:

$$\varepsilon = K_1 \sigma (F - F_0) \qquad (18)$$

WhereF, F_0 are the current and initial volume fractions of the β-phase respectively[18]. Then the strain rate is:

$$\dot{\varepsilon} = K_1 \sigma \dot{F} \qquad (19)$$

$\dot{F}$ is the β-phase volume fraction changing rate and it can be described using the chemical rate equation [18]:

$$\dot{F} = A \exp\left(-\frac{Q}{RT}\right)\left(F_{eq} - F\right)^n \qquad (20)$$

in which A is constant,F_{eq} is the equilibrium volume fraction of β-phase. It may be accurate to use $\frac{\varepsilon}{\sigma}$to estimate F in the above equation when the stress σ is constant, but if σ is varying with time, the linear relationship between the strain $\varepsilon$and $(F - F_0)$no longer exists. In an extreme case, where the stress σ decreased to zero during the phase change, the predicted strain rate is infinite. To apply equation (17) to a situation where both the temperature and the stress are changing with time, which is very likely during a transient,the creep strain rate equation is modified by the authors to account for the varying of stress:

$$\dot{\varepsilon} = 8 \times 10^{10} \sigma(t) * \exp\left(-\frac{26670}{T(t)}\right)\left(K_2 - \frac{\varepsilon_c}{\sigma_c}\right)^{2.4} \qquad (21)$$

where ε_c is the strain caused by constant stress σ_c under the same temperature transient $T(t)$, i.e.

$$\varepsilon_c = \int_0^t \dot{\varepsilon}_c \, dt = \int_0^t \left[8 \times 10^{10} \sigma_c * \exp\left(-\frac{26670}{T(t)}\right)\left(K_2 - \frac{\varepsilon_c}{\sigma_c}\right)^{2.4}\right] dt \qquad (22)$$

This is based on the fact that the rate of change of volume fraction of beta phase is independent of the applied load and is only a function of temperature.

2.2.3 Boundary conditions

For PT sagging problem, the support reactions at two fixed ends and the four garter springs are unknown. Six equations are thus needed to solve for these six unknowns. The two ends are assumed to be fixed, i.e. no axial displacement or rotation is allowed; the supports from garter springs are assumed to be rigid. Thus, the six boundary conditions can be expressed as follows:

$$\Delta\theta = \int_0^L K_{el}(x,t) + K_{pl}(x,t)\, dx = 0 \qquad (23)$$

$$\Delta y_i = \int_0^{Li} \left[K_{el}(x,t) + K_{pl}(x,t)\right](L_i - x) dx = 0 \quad i = 1,2,3,4,5 \qquad (24)$$

Equation (23) simply means the change of slope from one end to the other is zero, while equation (24) means no vertical displacement is allowed at the garter springs as well as at the two ends. $L_{1,2,3,4}$ are the distances from four garter springs to the left end, while L_5 is the distance from the right end to the left ($L_5 = L$). With the six support reactions, the bending moment at any location along the PT, i.e. $M(x)$ can be determined. The curvatures due to elastic and plastic strain are then calculated using equation (13 to 15) and deflections are found by integrating the curvatures along the axial direction.

2.3Model for the sagging of uncovered channel–"SAGCH"

"SAGCH" models the sagging of an uncovered channel, and it is only called when the CT temperature is sufficient for plastic deformation. To simply the model, it is assumed the PT and the CT sag together, i.e. the PT and the CT are simplified as one beam with two fixed ends under uniform distributed loads. The same beam theory and the same creep strain rate equation as "SAGPT"are used. The supporting forces at two fixed ends are solved before the deflections of the channel are calculated. Similarly, two boundary conditions are used: first, the tangents to the curve at both ends are horizontal; second, the deflections at two ends are zero.The first boundary condition can be interpreted as follows:

$$\Delta\theta = \int_0^L K_{el}(x,t) + K_{pl}(x,t)\, dx = 0 \qquad (25)$$

i.e. the change of slope from one end to the other is zero. The second boundary condition is:

$$\Delta y = \int_0^L \left[K_{el}(x,t) + K_{pl}(x,t)\right](L-x)dx = 0 \qquad (26)$$

i.e. the change of elevation from one end to the other is zero.

2.4 Coupling scheme

2.4.1 External Coupling – RELAP5/Mod3.3

A Python script which takes advantage of the "strip" and "restart" options of RELAP5 has been developed to externally couple the above described mechanistic PT deformation models with RELAP5/Mod3.3. Figure 2 shows the flow chart of the script.

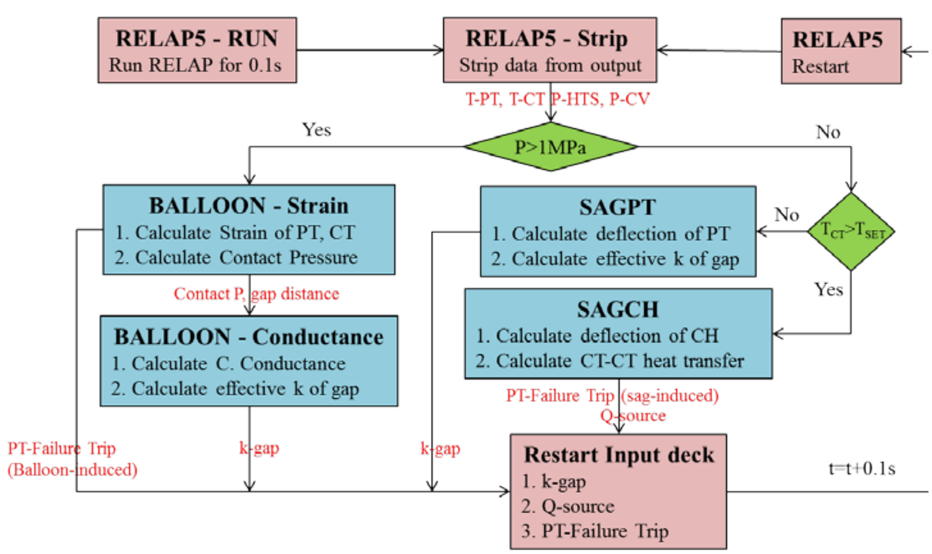

Figure 2 Flow chart of script for coupling

To allow coupling, the RELAP5 input deck is modified as follows:

1) A three-layer heat structure is used to represent the PT-CO_2-CT;
2) The material properties of the annulus (CO_2) are set as constant so they can be easily updated;
3) External heat sources are added to the CT heat structure to model channel-to-channel heat transfer after CT-CT sagging contact and are updated each coupling step;
4) Trip valves are used to connect the hydraulic volumes of fuel channel and moderator; these valves remain closed untilthe PT mechanistic failure criteria are satisfied; the trip cards used to trigger the trip valves are also updated during each coupling step.

As shown in figure 2, the script starts with an initial run (for one time step) after which relevant data including the temperatures of PT and CT, the pressures of fuel channel and CV etc. are stripped from the “RELAP5 restart file” and written to a “strip file”. The script then uses the “strip file” data to calculate the PT creep strain (transverse and longitudinal). Experiments have shown that transverse strain (balloon) and longitudinal strain (sag) can be calculated separately [20]. For an internal pressure greater than 1MPa, PT ballooning is the dominant deformation mechanism, and the effect of PT sagging isneglected; while for pressure less than 1MPa, PT sagging is the dominant deformation mechanism and the effect of PT ballooning is neglected. However, the script can be modified to allow ballooning and sagging to occur at the same time as there is evidence that neglecting the effect of sagging during PT ballooning will lead to the overestimation of contact temperature (discussed later). The geometries and strain of PT and CT are stored as global variables in Python, and are shared among the three models, i.e. “BALLOON”, “SAGPT” and “SAGCH”. To account for the reduced heat resistance across the annulus gap during ballooning or sagging, the effective conductivity (k) of the annulus region is updated based on the latest PT-CT geometriesand is updated during each coupling step.

<u>2.4.2 Internal Coupling – the Modified RELAP/SCDAPSIM/Mod3.6</u>

The above external coupling method is limited by the characteristics of RELAP5 heat structure, i.e.the RELAP5 heat structure only solves the heat conduction equations in the radial direction. PT-CT ballooning/sagging contact usually occurs earlier at axial location where the PT temperature is the highest, and after contact the local PT temperature drops rapidly if the CT is still submerged and sufficiently cooled. The subsequent steep temperature gradient makes axial conduction important. Meanwhile, if one heat structure is used to represent the PT-CT in a fuel channel, the input annulus material properties are shared by all axial nodes of the heat structure which precludes the possibility of modeling local PT-CT contact heat transfer using the above method. To allow local PT-CT contact, it is necessary to increase the number of heat structures in each channelsuch that there are individual PT, CO2, CT heat structures for each node in each channel of the core. However such proliferation of heat structures is not practical for a full plant transient since the maximum number of heat structures is limited.

To resolve these issues, the above developed models are integrated into RELAP/SCDAPSIM/ Mod3.6 as new SCDAP subroutines and internal coupling within RELAP is performed. SCDAP/RELAP5 is an integration of the RELAP5 code for thermal-hydraulics, SCDAP code for severe accident phenomena, and COUPLE code for lower vessel problems. The RELAP/SCDAPSIM code is being developed as part of the international nuclear technology program called SDTP. The as received version of RELAP/SCDAPSIM, Mod3.6 is being developed at Innovative Systems Software (ISS) to support the analysis of Pressurized Heavy Water Reactors (PHWRs) under severe accident conditions. The benefit of combining these mechanistic models with Mod3.6 is substantial. The SCDAP core components have many advantages over the RELAP5 heat structures: itsolves two-dimensional heat conduction equations in both radial and axial directions; it has additional severe accident models to modelmaterial oxidation, cladding deformation, fuel rod liquefaction and relocation and other severe accident phenomena; several additional PHWR specific modeling improvements have already been implemented in Mod3.6 [21].

To implement the three mechanistic models in Mod3.6, some changes have been made to both the code and the models (partial list):

1) New subroutine “ballon” is added to model the ballooning of PT and to calculate contact conductance across the annulus if PT/CT contact has been made. The temperature and pressure above which “ballon” is called can be user-input, in addition to inputs related to the PT failure strain.
2) New subroutine “sagpt” models the sagging of PT and determines PT/CT sagging contact. Currently, the number of garter springs is limited to four (typical CANDU fuel channel), but their locations can be user input. The additional user-input parameters include: the number of cells this PT is discretized into, the PT temperature above which this subroutine is called, and the loads applied to this PT.
3) New subroutine “sagch” models the sagging of a channel assembly, determines channel-to-channel contact, and calculates contact heat transfer. The temperature above which “sagch” is called, the applied load, the elevation of the channel (to determine CT-CT contact), the contact area, and the contact conductance can be user-input.
4) The subroutine to calculate effective material properties and effective volumetric heat generation for the shroud component is modified to account for the decrease in annulusheat resistance during PT ballooning. The contact conductance calculated by “ballon” and “sagpt” at/after PT-CT ballooning/sagging contact is converted to effective annulus conductivity in this subroutine.The channel-to-channel heat transfer calculated by “sagch” is converted tovolumetric heat generation and is also included in this subroutine.

3. Model Benchmark

In this section, the three mechanistic models are benchmarked separately against different experiments.All the data used for comparison are recorded before or at PT-CT contact. Thus, it is not necessary to model the transient after contact, and the temperatures are directly fed to the models to calculate the strain and/orthe deflections of the pipes. Some of the tests are repeated using the modified SCDAP/RELAP5code to confirm that all the new subroutines have been input correctly. SCDAP/RELAP5 allows user to define the temperature history for the SCDAP core components (although limited to uniform distribution). This greatly simplifies the validation process.

3.1 BALLOONBenchmark

3.1.1 Test 1 - PT temperature at contact

The first experiment used to benchmark“BALLOON” was conducted by Gillespie et al. [20]. In their experiments, a 3m long PT segment was contained in the 3m long CT and was internally heated by 26 electric heaters. The CT was then immersed in a water tank. The PT was supported by the two rolled joints at two ends and was separated from the CT by two garter springs. The PT was internally pressurized using helium. At the start of the test, the PT was first heated to 350°C. After holding it at this temperature for 10mins the power of the heaters was increased to obtain a linear temperature ramp at the center plane of the PT.The PT temperatures at contact were recorded as shown in table 2. Only the tests with internal pressure greater than 1MPa are selected. The predicted contact temperatures by BALLOON and SCDAP/RELAP5 are summarized in table 2, and the results predicted by TRAN II code are also included for comparison.

Table 2 Measured and predicted contact temperature for benchmark test 1

P (MPa)	Heat-up rate (°C/s)	Measured Contact T (°C)	BALLOON		SCDAP		TRAN II code [20]	
			Predicted(°C)	Error (°C)	Predicted (°C)	Error (°C)	Predicted(°C)	Error (°C)
1.0	2.0	735	794	59	796	61	797	62
1.0	2.4	760	801	41	803	43	804	44
2.0	4.0	750	775	25	774	24	764	14
4.0	5.6	720	744	24	743	23	743	23
4.0	4.5	710	736	26	736	26	720	10

The contact temperatures predicted by BALLOON are very close to those predicted by TRAN II (table 2),and as expected, the results predicted by SCDAP/RELAP5 and BALLOON are almost identical. The predicted contact temperatures in all the cases are overestimated especially when the pressure is low. This is attributed to the sagging of PT. In reality, the PT will also sag while ballooning radially towards the CT. Neglecting the effect of PT sagging will lead to a delayed PT-CT contact (thus higher contact temperatures).

3.1.2   Test 2 – PT temperature at failure

Another series of experimental tests which were conducted under CANDEV at Ontario Hydro Research Laboratories [4] are used to benchmark BALLOON. These tests were originally designed to validate the code NUBALL mentioned earlier. Since BALLOON is a uniform-temperature PT ballooning model, only the low temperature gradient tests are selected since large azimuthal gradients lead to non-uniform creep.In these tests, PT segments of 0.6m long were pressurized by either inert gas or steam. The variation of temperature around the circumference was of the order of 50°C. The PT heat-up rate was in the range 1-25°C/s with the internal pressure up to 5MPa. The temperatures at which very rapid straining of the PT occurs were taken as the failure temperature of PT.

The failure temperatures predicted by BALLOON are shown in figure 3, and the results predicted by NUBALL [4] are also plotted for comparison. In “BALLOON”, the PT is assumed to fail when the average creep strain exceed a user-input value. To be consistent with NUBALL, the PT failure strain in this test is set at 100%. The predicted failure temperatures by BALLOON agree well with the data from experiments, and failure curves predicted by BALLOON almost fall onto those predicted by NUBALL. It is also noted the predicted failure temperature is not sensitive to the used failure criteria due to the accelerated strain prior to the failure. The degree of the agreement illustrated in figure 3 can be achieved by using any average failure strain higher than 20%. This confirmed that the used failure criterion, i.e. an average creep strain of 20%, is reasonable when no severe circumferential temperature distribution is present.

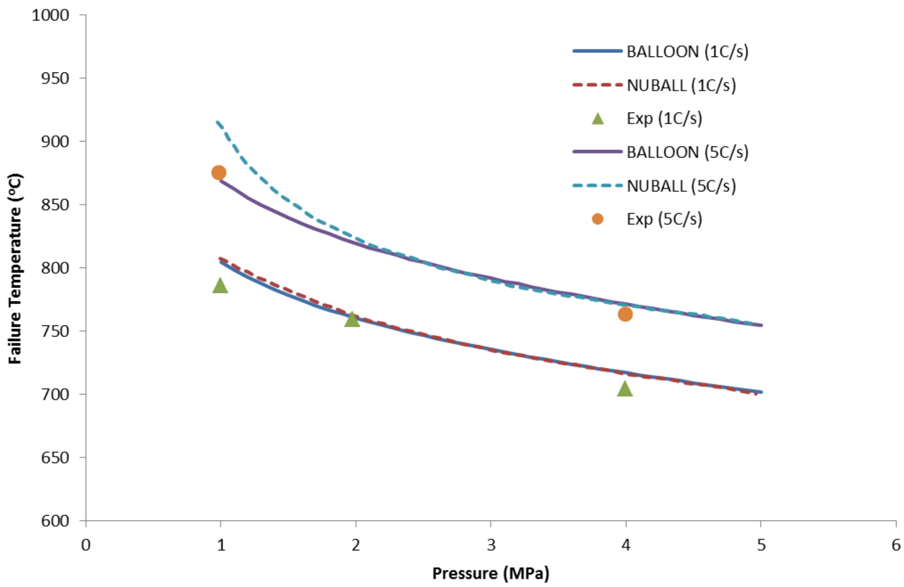

Figure 3Predicted failure temperatures at different heat-up rates

3.2 SAGPTBenchmark

To benchmark“SAGPT”, a different set of experiments by Gillespie et al. [22]is used. In these experiments they used a similar experimental apparatus design as in [20] except that the PTs were not pressurized. A 3m long PT segment was rolled into the end fittings at two ends. The heaters and other materials in the PT had the same weight per meter as CANDU fuel bundles.Thermo-couples were spot-welded to the surface of PT to record temperature. The power of the heaters was varied to obtain a linear temperature ramp. LVDTs (Linearly Varying Deflection Transformers) were used to record the deflections of the PT. The PT was surrounded by a 30 mm air gap and then by solid insulation.

In this benchmarktest, the “SAGPT” is modified to represent the experimental apparatus: the gap distance between PT and CT is increased to 30mm and the length of the PT changed to 3 m; some of the garter springs are “removed”. The PT temperature as a function of deflection is calculated. Due to the lack of information from reference [22], the heatup rates along the PT are assumed to be uniform. However, in reality the heat up rates at two ends are expected to be lower than the center due to heat loss byaxial heat conduction. The sensitivity to the temperature uniformity is thus investigated for test 3.1 and 3.2. Table 3 summarized the experimental conditions of each test as well as the measured and predicted PT temperatures. The predictions by code “CREEPSAG”[22] are also included for comparison.“CREEPSAG” is developed by AECL to analyze the bending deflection of a PT. Unless otherwise noted,the results predicted by SAGPT and SCDAP in the following table are based on uniform-temperature assumption.

Table 3Measured and predicted PT temperature at given deflections

Exp	Temp. Ramp (°C/s)	Spacer Loc. (m)	LVDT Loc. (m)	Measured Temp. (°C)	SAGPT (°C)	SCDAP (°C)	CREEPSAG (°C)[22]
3.1	3.0	-	1.5	820[a]	794 (821[d])	797	800
3.2	2.7	-	1.5	810[a]	790 (816[d])	790	830
3.3	3.3	1.5	1.0	890[b]	917	-	880
3.4	3.1	1.5	1.0	820[b]	911	-	940
3.5	2.8	1.5	1.0	860[b]	900	-	890
3.6	3.0[c]	-	1.5	890[a]	900	-	870

a Deflection is 20mm
b Deflection is 10mm
c Varied from 2.8 to 3.4°C/s along the tube
d At both ends the PT heatup rates are assumed to be 80% of the center over a length of 0.25m

In tests where the spacer was not used, i.e. test 3.1, 3.2 and 3.6, the temperatures predicted by “SAGPT” agree well with the experimental data. The underestimation of results in test 3.1 and 3.2 is attributed to the uniform-temperature assumption used. Sensitivity studies show that if the heatup rates at two ends are lowered by 20% to account for the heat loss due to axial conduction, the predicted temperatures become much closer to the measured ones (table 3).

In tests where the spacerwas used, the temperatures are significantly overestimated especially in test 3.4. This is attributed to the rigid garter spring (spacer) assumption used in “SAGPT”. In the experiments the PTswere found to have deformed locally at the spacers, and the spacers also buckled, while in “SAGPT” the spacer geometry is invariant. “CREEPSAG” also showed the same behavior as “SAGPT”.

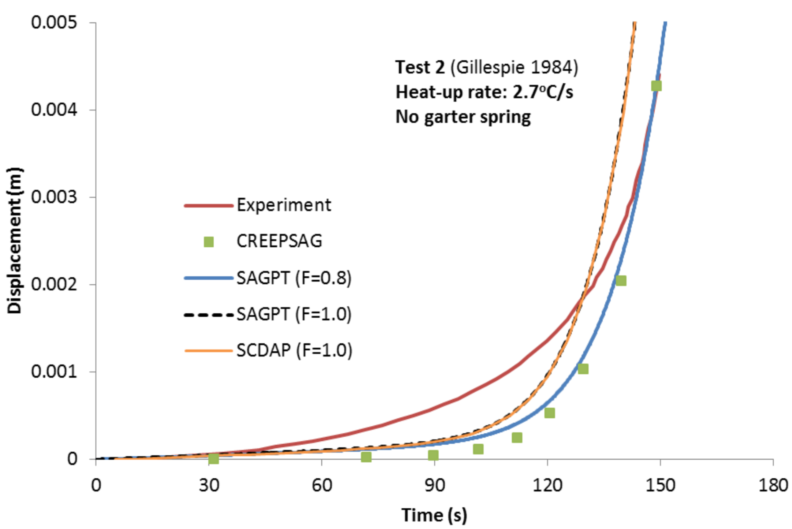

Figure4 Measured and predicted displacement at LVDT in test3.2
(F=1.0: uniform temperature; F=0.8: heatup rate at two ends is 80% of the center)

Figure 4 shows the measured and predicted displacements at the LVDT (1.5 m) in test 3.2. It can be seen that if the temperature along the pipe are assumed to be uniform, the predicted displacement at the center increases much faster than the measured one and that predicted by CREEPSAG. However, the results show large sensitivity to the temperature variation at two ends.

If the heatup rates at two ends are lowered by 20% (over a length of 0.25m at both ends), excellent agreements between the curves predicted by "SAGPT" and "CREEPSAG" are observed. All the models show large discrepancies between the measured and predicted results during the first 100s. This is attributed to the same creep strain rate equation used in these models. It is likely that Equation (17) is under-predicting the creep strain rate below 700°C. However, as temperature increases the creep strain rate increases rapidly. The initial discrepancies thus become less important.

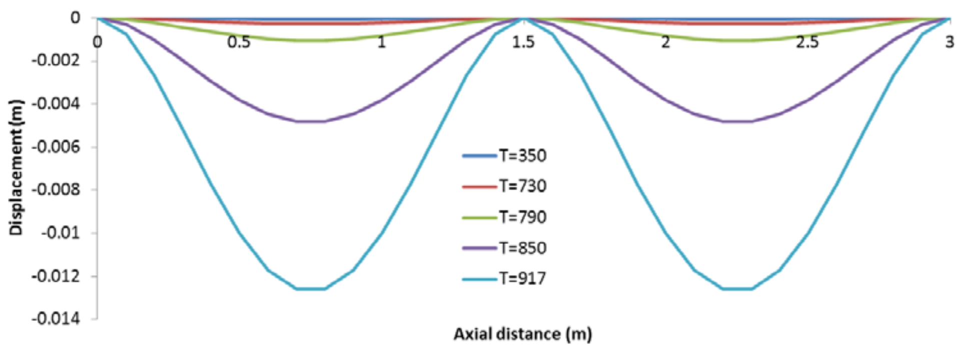

Figure5PT profile predicted by SAGPT during the temperature ramp in test3.3

Figure 5 shows the predicted PT profile in test 3.3. The deflections of PT arenegligiblewhen temperaturesare below 700°C and increase rapidly at temperatures around 850°C. In this test the LVDT was located at 1 m. SAGPT predicts a PT temperature of 917°C when the deflectionat LVDT reaches 10 mm (slightly higher than the measured temperature). In SAGPT if the PT is allowed to deform at the spacers (x = 1.5m), the results are expected to be much closer to the experimental data. A mechanistic spacer deformation model is thus needed.

In test 3.6 an axial temperature gradient was imposed by varying the heat-up rate along the PT. The imposed temperature at one end (x = 0m) was higher than that at the other end (x = 3m) resulting in asymmetric PT deflections. The displacements of the PT at various locations at the time of 212swere recorded. The measured and predicted PT profilesare shown in figure 6. The magnitude and location of the maximum displacement are well predicted by SAGPT, while thedeflections on the right side are underpredicted. It is suspected that inconsistent experimental conditions are used due to the lack of information fromreference[22].

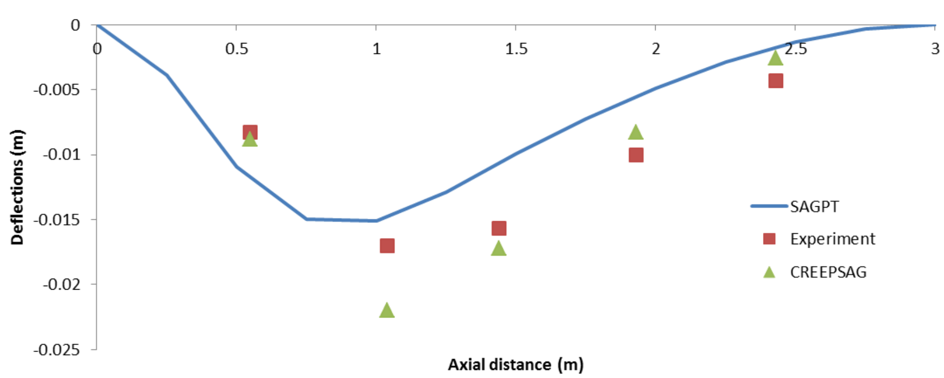

Figure 6Measured and Predicted PT deflections at 212 seconds in test3.6

3.3 SAGCH Verification

SAGCH has not been explicitly validated due to the lack of relevant experimental data from open literature, but it has been verified by simply modifying the geometries of the channel in the model to represent a PT with no support from the spacers such as those in test 3.1, 3.2. Thesetests were repeated to ensure that consistent results are predicted by SAGCH.

The experimental data from the core disassembly test facility (CDF) [23]at AECL is ideal for the future validation of SAGCH. In CDF, the CANDU fuel channel is scaled down to a one-fifth linear scale while maintaining the same stress level at the channel center plane. The test results showed significant strain localization at the bundle junctions along the bottom side of the channel[23]. Thus special treatment may be needed in SAGCH to account for this stress concentration.

4. Conclusion and future work

Three mechanistic channel deformation models which can be coupled with thermal-hydraulic code RELAP5 have been developed to model the PT ballooning/sagging and the channel sagging in a postulated accident of CANDU reactors. A Python script has been developed to externally couple these models with RELAP5/Mod3.3 in which the PT-CO_2-CT is represented by a RELAP5 heat structure. The models have also been integrated into RELAP/SCDAPSIM/Mod3.6 as new SCDAP subroutines to overcome the RELAP5 limitations on heat conduction and material properties. The detailed descriptions of the models and the two different coupling schemes are presented in this paper. The models were benchmarked against several PT deformation experiments. The model predictions agreed well with the experimental data.

However, for the PT ballooning model “BALLOON”, it is found the model over-predicted the contact temperature especially when the internal pressure was low. This is mainly because at the current stage of development “BALLOON”is not coupled with the PT sagging model (PT deflection due to sagging is neglected under high pressure conditions), while in reality the PT will also sag while expanding radially towards the CT. The time to contact is thus overestimated as well as the contact temperature. “BALLOON” was also used to predict the PT failure temperatures in experimental tests with different heat-up rates and internal pressures up to 5MPa. For tests with small circumferential temperature gradient, any average creep strain higher than 20% is found to predict the failure temperatures quite well due to the accelerated strain prior to the failure.

The sagging models “SAGPT” were used to model several low-pressure PT deformation tests. In tests where the garter springs or spacers were used, the models were found to overestimate the temperatures at given deflection (or at PT-CT contact). This is because in the current model the spacers are assumed to be rigid, i.e. they are not allow to move or deform, while in experimentsthey were found to have buckled under high temperatures. To better predict PT sagging, a mechanistic spacer deformation model is thus needed.

Reference

[1] R. S. W. Shewfelt, L. W. Lyall, and D. P. Godin, "A HIGH-TEMPERATURE CREEP MODEL FOR Zr-2.5 wt% Nb PRESSURE TUBES," *J. Nucl. Mater.*, vol. 125, pp. 228–235, 1984.

[2] R. S. W. Shewfelt, D. P. Godin, and L. W. Lyall, "Verification of High-Temeprature Transverse Creep Model for Zr-2.5 wt.%Nb Pressure Tubes," *AECL Rep. 7813*, 1984.

[3] R. S. W. Shewfelt and D. P. Godin, "Verification Tests for GRAD, A Computer Program to Predict the Non-uniform Deformation and Failure of Pressure Tubes During a Postulated LOCA," no. March, 1985.

[4] P. Kundurpi, "Validation of Computer NUBALL for Simulation of Pressure Tube Asymmetric Ballooning Behaviour," in *2nd International on Simulation Method in Nuclear Engineering*, 1986.

[5] Q. M. Lei and H. Z. Fan, "An Improved Model to Predict Nonuniform Deformation of Zr-2.5 NB Pressure Tubes," 1997.

[6] R. S. W. Shewfelt, "Ballooning of CANDU Pressure Tubes - Model Assessment," *Res. Rep. AECB*, 1990.

[7] G. E. GILLESPIE, "An experimental investigation of heat transfer from a reactor fuel channel to surrounding water," in *2nd Annual CNS Conference*, 1981.

[8] J. C. Luxat, "Mechanistic Modeling of Heat Transfer Processes Governing Pressure Tube-To-Calandria Tube Contact and Fuel Channel Failure," in *23rd CNS annual conference*, 2002, pp. 1–26.

[9] A. Cziraky, "Pressure Tube-Calandria Tube Thermal Contact Conductance," *McMaster Master Thesis*, 2009.

[10] M. M. Yovanovich, "Micro and macro hardness measurements, correlations, and contact models," *44th AIAA Aerosp. Sci. Meet. Exhib.*, no. January, pp. 1–28, 2006.

[11] P. Neal and C. Fraser, "Contact Boiling Experiement SUBC3," *COG-02-2018*, 2003.

[12] H. Z. Fan, Z. Bilanovic, and T. Nitheanandan, "Use of CATHENA to Model Calandria-Tube/Moderator Heat Transfer After Pressure-Tube/Calandria-Tube Ballooning Contact," in *CNS 6th International Conference on Simulation Methods in Nuclear Engineering*, 2004, pp. 1–13.

[13] S. M. Petoukhov, "MAAP4-CANDU Analysis of a Generic CANDU 6 Station: Preliminary Results for a Large LOCA Scenario," in *23rd CNS annual conference*, 2002, pp. 1–15.

[14] IAEA, "Analysis of Severe Accidents in Pressurized Heavy Water Reactors," *TECDOC 1594*, no. June, 2008.

[15] D. Dupleac, M. Mladin, and I. Prisecaru, "Generic CANDU 6 plant severe accident analysis employing SCAPSIM/RELAP5 code," *Nucl. Eng. Des.*, vol. 239, no. 10, pp. 2093–2103, Oct. 2009.

[16] R. S. W. Shewfelt and L. W. Lyall, “A High-Temperature Creep Model for Zircaloy-2 Calandria Tubes,” *COG-88-37*, 1988.

[17] R. S. W. Shewfelt and D. P. Godin, “The Effect of Axial Scratches on the Ductile Creep Rupture of Internally Pressurized Thin-Walled Tubes,” *Res Mech.*, vol. 13, pp. 1–13, 1985.

[18] R. S. W. Shewfelt, L. O. N. D. Nal, and L. W. Lyall, “A High-Temperature Longitudinal Strain Rate Equation For Zr-2 . 5 wt % Nb Pressure Tubes,” *J. Nucl. Mater.*, vol. 132, pp. 41–46, 1985.

[19] M. De Jong and G. . Rathenau, “Mechanical properties of iron and some iron alloys while undergoing allotropic transformation,” *Acta Metall.*, vol. 7, no. 4, pp. 246–253, 1959.

[20] G. E. Gillespie and G. I. Hadaller, “An experimetnal investigation into the development of pressure tube/calandria contact and associated heat transfer under LOCA condition,” in *CNS 6th Annual Conference*, 1985.

[21] A. Bonelli, O. Mazzantini, D. Dupleac, and E. Dinca, “RELAP / SCDAPSIM / MOD3 . 6 – Development of Severe Accident Models for Heavy Water Reactors Including CANDU and ATUCHA-2,” 2015.

[22] G. E. Gillespie and R. G. Moyer, “An experimental invetigation of the ceep sag of pressure tubes under LOCA conditions,” in *CNS 5th Annual CNS Conference*, 1984.

[23] P. M. Mathew, a J. White, V. G. Snell, and M. Bonechi, “Severe Core Damage Experiments and Analysis for CANDU Applications,” in *SMiRT 17*, 2003, pp. 1–8.