PREDICTION OF THE FUEL FAILURE FOLLOWING A LARGE LOCA USING MODIFIED GAP HEAT TRANSFER MODEL

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ABSTRACT

The modified Ross and Stoute gap heat transfer model in the ELOCA.Mk5 code for CANDU safety analysis is based on a simplified thermal deformation model. A review on a series of recent experiments reveals that fuel pellets crack, relocate, and are eccentrically positioned within the sheath rather than solid concentric cylinders. In this study, more realistic offset gap conductance model is implemented in the code to estimate the fuel failure thresholds using the transient conditions of a 100% Reactor Outlet Header (ROH) break LOCA. Based on the offset gap conductance model, the total release of I-131 from the failed fuel elements in the core is reduced from 3876 TBq to 3283 TBq to increase margin for dose limit.

1. INTRODUCTION

In CANDU safety analysis, ELOCA.Mk5⁽¹⁾ transient fuel behaviour simulations are used to calculate the thermo-mechanical response of a fuel element and fission product releases during the accident. The dynamic gap conductance model in the ELOCA.Mk5 code assumes a modified Ross and Stoute model^{(2),(3)} based on a simplified thermal deformation model. This model is lower bound approach and hence conservative only in terms of fuel surface temperature predictions (i. e., initial stored energy) for normal operation conditions. The amount of stored energy in the fuel at the start of a reactor transient plays an important role in the response of the fuel element during the transient. The sheath temperature after dryout could be underpredicted based on the modified Ross and Stoute model. Therefore, for transient conditions, relationship between gap heat transfer and fuel failure is very complicated and more realistic gap model is required.

The mechanism that governs heat transfer across the fuel-sheath gap has been well understood⁽⁴⁾. One significant trend in thermal calculations in the past ten years has been a steady reduction in calculated values for fuel temperatures and stored energy⁽⁵⁾. This perspective permitted data interpretation and fuel element modeling to focus on effective gap size rather than on the gap conductance mechanism itself. U.S. NRC Regulatory Guide⁽⁶⁾ recommends that the calculation of the gap width during reactor operation (hot gap size) take into account UO₂ fuel swelling, densification, creep, thermal expansion and fragment relocation, and sheath creep. The recently-proposed models such as offset gap conductance model^{(7),(8),(9)} and relocated gap conductance model⁽¹⁰⁾ include the above essential phenomena and are based on in-pile and out-of-pile test data. As a result, the heat transfer across the fuel-sheath gap is significantly greater than what is calculated with fuel pellet modelling as solid concentric cylinder.

In this paper, the recently-proposed, more realistic offset gap conductance model is described along with the modified Ross and Stoute model. For verification purpose, the model is applied to calculate the fuel-sheath gap conductance under the conditions of experiment. Fuel failure calculations following a 100% Reactor Outlet Header (ROH) break LOCA are also performed for an estimate of I-131 release transients.

2. DESCRIPTION OF GAP CONDUCTANCE MODELS

The international nuclear community has used the work of Ross and Stoute^{(2),(3)} as a standard, classical reference for fuel-to-sheath heat transfer; essentially all of the present fuel-to-sheath heat transfer models are based to some extent on their correlations. The modified Ross and Stoute model is incorporated in ELOCA.Mk5. The offset gap conductance model has been incorporated into state-of-the-art calculation methods for fuel element thermal response (FRAP-T6⁽⁷⁾, RELAP5⁽⁸⁾, and GAPCON-THERMAL-2⁽⁹⁾).

2.1 Modified Ross and Stoute Model

Thermal conductance of the fuel-sheath gap is a strong function of hot gap size and of the composition and pressure of the gases in the fuel element. The thermal conductance of the fill gas/fission gas mixture at the fuel-to-sheath interface is given by

$$hf = \frac{kg}{1.5 (R_1 + R_2) + tg + g}$$
(1)

Where,	hf	=	conductance through the gas in the gap $(W/cm^2 \cdot K)$
	kg	=	thermal conductivity of gas (W/cm K)
	R_1, R_2	=	surface roughnesses of the fuel and the sheath (cm)
	tg	=	circumferentially averaged fuel-sheath gap width (cm)
	g	=	temperature jump distance as a function of gas temperature, pressure,
			and composition

2.2 Offset Gap Conductance Model

The offset gap conductance model correctly predicts the significant circumferential variation in fuel temperature that was measured during the test series. The model is consistent with test results indicating that fuel pellets are offset from the sheath center-line instead of centrally located within the sheath. This variation causes the conductance through the gas in the gap to vary with circumferential position. The circumferential variation of the conductance is taken into account by dividing the gap into several equal segments. The conductance for each segment is calculated and then an average conductance is computed.

The temperature jump distance terms account for the temperature discontinuity caused by incomplete thermal accommodation of gas molecules to the surface temperature. The terms also

account for the inability of gas molecules leaving the fuel and sheath surfaces to completely exchange their energy with neighboring gas molecules, which produces a nonlinear temperature gradient near the fuel and sheath surfaces. The terms are calculated by

$$g' = 0.024688 \left[\frac{k_g T_g^{-1/2}}{P_g \sum_{i} y_{iai} M_i^{-1/2}} \right]$$
(2)

Where, $a_i = accommodation coefficient of the i-th component of gas$ $M_i = molecular$ weight of the i-th component of gas

The accommodation coefficients for gases are obtained by using curve fits to the data of Ullman⁽¹¹⁾.

3. APPLICATION OF GAP CONDUCTANCE MODELS

3.1 Experiment Simulation

Results of the experiment⁽³⁾ performed previously were used to assess the applicability of the offset gap conductance model implemented in ELOCA.Mk5 code to in-reactor conditions. Campbell et al. performed a series of instrumented in-reactor measurements in which the fill gas composition and pressure were controlled. Variations in fuel temperature and sheath strain were determined as the internal gas pressure of helium or argon was varied. During these pressure cycles, the pressure was varied in steps with the size of each step more or less proportional to pressure. These experiments showed that where there was a fuel-to-sheath gap, the width of which could be calculated from the change in sheath strain and fuel expansion, the classical approach of Ross and Stoute based on laboratory measurements agreed closely with experiment.

Comparison with experimental data of heat transfer through the fuel-sheath gap was conducted to ensure that the offset gap conductance model performed correctly in ELOCA.Mk5. As shown in Figure 1, the good agreement between the experimental and calculated values demonstrates that the offset gap model has been implemented correctly. The offset gap conductance model correctly predicts the significant circumferential variation in fuel temperature that was measured during the test series (using 3 thermocouples). The model is consistent with test results indicating that the width of the fuel-sheath gap varies with circumferential position. Furthermore, this discrepancies of fuel surface temperatures become more pronounced with increasing gap size for the recently-proposed model due to pellet eccentricity. Therefore, the effect of this realistic trend on temperature prediction is more important for transient condition rather than normal operating conditions.

3.2 I-131 Release Calculations Following a Large Break LOCA

To assess the effect of the gap heat transfer model on gap heat transfer, fuel behaviour following a large LOCA is simulated using the ELOCA.Mk5 computer code. Fuel behaviour is

simulated using thermohydraulic boundary conditions from the CATHENA single-channel simulations and the power transients following a large LOCA. Transient fuel behaviour of temperature, pressure, sheath strain and heat transfer is simulated using the steady-state conditions from ELESTRES_M11C runs following the overpower envelope. A 100 percent Reactor Outlet Header (ROH) break is selected as a critical break which results in the largest number and earliest timing of fuel failures. The analysis is performed using the methodology-identical to that described in the Final Safety Analysis Report⁽¹²⁾.

Thresholds for Fuel Failure. The fuel failure thresholds are defined as follows: for a given burnup, the fuel failure threshold is the minimum linear power which would result in a prediction of fuel element failing following a 100% ROH break. Simple and conservative criteria are used to determine whether a fuel element fails or not, based on the predictions of the ELOCA.Mk5 code. These criteria are based on experimental data and experience with operating reactors.

Transient I-131 Release from Failed Fuel Elements. This part of the analysis makes use the results of the fuel failure threshold calculation and the ELOCA.Mk5 transient fuel behaviour simulations which were used to determine the failure thresholds. The fission product inventory which is available for release following the event depends on the configuration of element powers and burnups in the reactor core at the time of the accident. The powers and burnups of all the fuel bundles for 260 full power days are obtained to maximize the I-131 gap inventory⁽¹²⁾. In order to simplify the calculations, the fuel elements in the core are grouped according to their powers and burnups (using 29 power intervals and 24 burnup intervals). The number of fuel elements expected to fail is estimated by adding up the number of elements in each power/burnup group where the power is equal to or greater than the fuel failure threshold at a specified burnup. An estimate of I-131 release is obtained by determining which fuel elements are expected to fail following the accident and their times of failure. Gap inventory is assumed to be released immediately when the fuel elements fail. One percent of the grain inventories is added to the releases to account for the possibility of additional releases of fission products from the fuel matrix due to diffusion, oxidation, Zircaloy-UO₂ interaction and UO₂ cracking.

4. RESULTS AND DISCUSSION

Typical fuel behaviour following a 100% ROH break is shown in Figures 2 and 3 for an element in the outer ring at the top of bundle 6 in channel O6_mod. The fuel element burnup at time of accident is assumed to be 150 MW h/kg(U)). After 30 seconds, the discrepancy of the gap width and the gap heat transfer become more pronounced for the offset gap conductance model due to the enhanced eccentricity of gap. The difference between the resulting sheath strains calculated based on the modified Ross and Stoute, and offset gap models increases depending on the gap width, i. e., heat transfer from the UO₂ to the sheath. The fuel element is predicted to fail at 55 seconds for the modified Ross and Stoute model and at 64 seconds for the offset gap model. In transient thermal calculations, lower values of heat transfer across the fuel-to-sheath gap give lower fuel sheath temperatures at the same initial stored energy, especially in wide-gap region (higher than ~ 500 μ m).

4.1 Thresholds for Fuel Failure

The limiting fuel failure mechanisms for the 100% ROH break are determined as follows:

- i. Excessive diametral strain; the fuel sheath fails if uniform sheath strain exceeds 5% for sheath temperatures below 1000°C^{(13),(14)}.
- ii. Significant cracks in the surface oxide; the fuel sheath fails if the uniform sheath strain exceeds 2% for sheath temperatures above $1000^{\circ}C^{(15)}$.

During the high temperature transient these two failure mechanisms are used to determine the failure threshold power. Significant diametral strain is predicted for high and intermediate burnup fuel elements, however fuel sheath temperatures remain below 1000°C. Therefore, only for the high-power (i. e., high-temperature) and low-burnup elements, the failure criterion of 2% plus sheath temperature in excess of 1000°C is limiting. The elements at the burnups lower than 120 MW·h/kg(U) are predicted to fail earliest about 27 seconds after the event by 2% criterion on the basis of the modified Ross and Stoute gap conductance model. In the case of offset gap model, the pellet eccentricity and light contact with the sheath reduce the calculated sheath temperature to remain below 1000°C.

The resultant fuel failure thresholds at different burnups are shown in Figure 4. With higher burnup, the fuel element fails at the power much lower than the limiting envelope. The pellet eccentricity increases the predicted sheath temperature and strain defect threshold for fuel failure at the burnups ranging from 50 MW·h/kg(U) to 110 MW·h/kg(U) and at the burnup of 150 MW·h/kg(U). Especilly, the highest discrepancy in the threshold occurs at the burnup of 60 MW·h/kg(U) due to the highest element power prior to the transient.

4.2 Transient I-131 Release from Failed Fuel Elements

Using the powers and burnups in the core, the number of failed fuel elements in the critical pass following a 100% ROH LOCA is 1206 based on the modified Ross and Stoute gap model. The number of failed elements predicted by the offset gap model is reduced to 1008 (about 10% decrease). Figure 5 shows total I-131 release from the critical pass. The fuel element behaviours predicted for I-131 release transients for both gap models are very similar with higher burnups because of the same thresholds. Especially, at the burnup of 110 MW·h/kg(U), since the fuel elements not failed are higher power (i. e., 48 kW/m to 51 kW/m) and have higher I-131 inventories, the discrepancy of the release is predicted to be higher than expected on the basis of the failure thresholds. Using the offset gap model, no fuel failures are predicted at the element burnups ranging from 60 MW·h/kg(U) to 90 MW·h/kg(U) because their differences of failure thresholds are higher. Therefore, most dominant factor in determining the I-131 release is the failure thresholds, which depend strongly on the gap heat transfer and sheath temperature during the transient.

The total release of I-131 is reduced from 3876 TBq to 3283 TBq, a difference of about 15% due to the pellet eccentricity and light contact with the sheath. The I-131 release transient following the 100% ROH is constructed by adding the releases from failed fuel at each second as shown in Figure 6. As well as total amount of the releases, the timing of the releases is predicted to be delayed

in the enhanced eccentric gap model relative to that in the modified Ross and Stoute model. At 32 seconds after the break, the first release is predicted to occur from the fuel element which belongs to the power/burnup group of a 52 kW/m and 150 MW·h/kg(U) combination.

Relocation quickly becomes complete in a fuel element. The fragment moves outward to lightly contact the sheath, creating an effective gap width. The offset gap conductance model correctly predicts the significant circumferential variation of fuel temperature that was measured during the test. As a result, the effective gap width and the calculated values for fuel temperatures and initial stored energy for normal operating conditions and then sheath temperatures during the transient are reduced. Therefore, the prediction of the physically-based, offset gap conductance model provides more realistic values for fuel-to-sheath gap heat transfer and fission product releases compared to the modified Ross and Stoute model.

Fission gas released from the pellet prior to the accident contaminates the original helium fill gas. Because fission gas is primarily xenon, with a conductivity 1/20 that of helium, fission gas reduces its conductivity, and raises the fuel temperature at constant element power. These effects produce more fission gas release, and the process continues until the fuel element stabilizes at the point that its fill gas is thoroughly saturated with fission gas ("thermal feedback"). If the pellet eccentricity reduce the temperature effect of varying gap size and fill gas composition at Beginning-of-life (BOL), then the phenomena could be expected to reduce the impact of "thermal feedback". The predicted I-131 release resulting from the thermal feedback with and without eccentricity is extreme; there is a spread of about 600 TBq between the highest and lowest predicted values of the releases as shown in Figure 6. End-of-life (EOL) burnups for LWR fuel are significantly higher than that for CANDU fuel. The "tuning" that improves LWR predictions based on the offset gap conductance model at EOL could be less effective under some conditions for the low burnups applicable to CANDU fuel at EOL.

5. CONCLUSIONS

- i. The offset gap conductance model in ELOCA.Mk5 correctly predicts the significant circumferential variation of fuel temperature measurements. The gap conductance model provides more realistic values for gap heat transfer and fuel surface temperatures compared to the modified Ross and Stoute model,
- ii. For a 100% ROH break LOCA, the pellet fragment eccentricity reduces the calculated values for initial stored energy and sheath temperatures during the transient. Effective gap width and the impact of "thermal feedback" caused by fission product released into the gap are reduced, and
- iii. Conservatism of the modified Ross-Stoute gap conductance model is verified for 100% ROH break in terms of dose calculations. Based on the enhanced eccentricity of gap, the timing of I-131 release is delayed, and the total release from the failed fuel elements is reduced from 3876 TBq to 3283 TBq to increase margin for dose limit.

6. REFERENCES

- (1) J.R. Walker, J.W. de Vaal, V.I. Arimescu, T.G. McGrady, D.C.K Wang and C. Wong, "ELOCA.Mk5: Theory Manual", AECL Research Report COG-92-001C/RC-667, 1992.
- (2) A. M. Ross and R. L. Stoute, "Heat Transfer Coefficient Between UO₂ and Zircaloy-2", AECL-1552, 1962.
- (3) F. R. Campbell, L. R. Stoute, R. Deshaies, H. Sills and M. J. F. Notley, "In-Reactor Measurement of Fuel-to-Sheath Heat Transfer Coefficients between UO₂ and Stainless Steel", AECL-5400, 1977.
- (4) J. E. Garnier and S. Begej, "Ex-Reactor Determination of Thermal Gap and Contact Conductance Between Uranium Dioxide: Zircaloy-4 Interfaces—Stage I: Low Gas Pressure", NUREG/CR-0330, PNL-2696, 1979 April.
- (5) G. A. Berna et al., "FRAPCON-2: A Computer Code for the Calculation of Steady State Thermal-Mechanical Behavior of Oxide Fuel Rods", NUREG/CR-1845, 1981 January.
- (6) U. S. NRC Regulatory Guide 1.157, "Best-Estimate Calculations of Emergency Core Cooling System Performance", 1989 May.
- (7) L. J. Siefken et al., "FRAP-T6: A Computer Code for the Transient Analysis of Fuel Rods", NUREG/CR-2148, EGG-2104, 1981 May.
- (8) Idaho National Engineering Laboratory, "RELAP5/MOD2 Code Manual", Vols. 1 & 2, NUREG/CR-4312, 1985 August.
- (9) C. E. Beyer et al., "GAPCON-THERMAL-2: A Computer Program for Calculating the Thermal Behavior of an Oxide Fuel Rod", BNWL-1898, 1978 November.
- (10) G. A. Berna et al., "Gap Conductance Test Series-2 Test Results Report for Tests GC 2-1, GC 2-2, and GC 2-3", NUREG/CR-0300, TREE-1268, 1978 November.
- (11) A. Ullman, R. Acharya and D. R. Olander, "Thermal Accommodation Coefficients of Inert Gases on Stainless Steel and UO₂", *Journal of Nuclear Materials*, 51, 1974, pp. 277–279.
- (12) "Large Breaks in the Primary Circuit with Containment and Emergency Core Cooling System Functions Available", Chapter 15, Wolsong 2/3/4 Final Safety Analysis Report, 1995.
- (13) AECL (M.R. Matthias) submission to AECB (J.P. Marchildon, B.M. Ewing), 1982 March 01 with attachment by E. Kohn, "Use of 5 Percent Uniform Strain for Activity Release Predictions".
- (14) C.E.L. Hunt, "The Limit of Uniform Strain, or Onset of Ballooning, in Fuel Sheath Ballooning Tests", AECL Report CRNL-1187, 1974 September.
- (15) S. Sagat et al, "Deformation and Failure of Zircaloy Fuel Sheaths Under LOCA Conditions", AECL-7754, 1982 October.



Figure 1. Fuel Surface Temperature Predictions with Experimental Measurements for Helium Pressure Cycle Experiments (Reference (3), AECL-5400)



in Channel O6_mod (150 MW·h/kg(U))



Figure 3. Strain Transients for an Outer Element at the Top of Bundle 6 in Channel O6_mod (150 MW·h/kg(U))





Time (s)

Figure 6. Transient I-131 Release for 103% Full Power Following a 100% ROH Break LOCA

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