

ELESTRES Code Upgrades

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1. ABSTRACT

The fuel-performance code ELESTRES (ELEment Simulation and sTRESSes) models the in-reactor and on-power behaviour of CANDU[®] fuel elements under normal operating conditions. The code also provides initial conditions for evaluating fuel behaviour during high-temperature transients. The CANDU fuel community uses the ELESTRES-IST (Industry Standard Toolset) version of the code to assess the performance of CANDU fuel designs (e.g., standard natural uranium CANDU fuel, CANFLEX[®] fuel, and low-void-reactivity fuel (LVRF)).

The CANFLEX fuel design is evolving to meet more demanding requirements, such as higher burnup operations and higher coolant temperatures and pressures, compared to the current CANDU fuel designs. LVRF uses a burnable poison, (U,Dy)O₂ in the central element of the CANFLEX bundle, to achieve lower void reactivity during a postulated loss-of-coolant accident. The ELESTRES code must be capable of simulating these more demanding CANDU fuel applications. A version of the ELESTRES code based on the ELESTRES-IST code version is under development to provide a tool that is qualified to model CANDU fuel performance under these more demanding reactor operating conditions.

This paper describes recent ELESTRES code capability upgrades. The paper identifies the key model enhancements, and the implementation, verification and validation activities that are being performed in accordance with the AECL software quality assurance program.

CANDU[®] (CANada Deuterium Uranium) is a registered trademark of Atomic Energy of Canada Limited (AECL).

CANFLEX[®] (CANdu FLEXible) is a registered trademark of AECL and the Korea Atomic Energy Research Institute (KAERI).

2. INTRODUCTION

The ELESTRES code performs calculations of the following major fuel performance parameters: temperature, fission-gas release, internal pressure, and fuel deformation. In arriving at these fuel performance calculations, the code considers a number of effects explicitly: for example, burnup-dependent neutron flux depression across the pellet radius; variation of pellet-to-sheath heat transfer coefficient with burnup; production, migration (including trapping and resolution), and release of stable and radioactive fission products; grain growth; grain boundary sweep; densification; fission-product swelling caused by grain boundary bubbles; thermal expansion; elasticity; plasticity; creep; and cracking of UO_2 ; and variation of material properties with temperature and with burnup.

For temperature distribution in the pellet and sheath, ELESTRES uses a two-dimensional finite element method. For fission-gas release and associated calculations, ELESTRES uses a microstructure-dependent model [1]. For pellet deformation, ELESTRES uses a two-dimensional axisymmetric finite-element method [2].

The ELESTRES-IST code is the industry standard tool for simulating the behaviour of CANDU fuel designs under normal operating conditions. It has been qualified for use with natural uranium fuel [3] in accordance with the AECL software quality assurance (SQA) program and Canadian Standards Association CSA-N286.7-99. There is a need to extend the range of application of the code to more demanding conditions, including higher burnup, higher coolant temperatures and pressures, and to model the performance of burnable poison $(\text{U,Dy})\text{O}_2$ fuel, used in the LVRF bundle [4] to lower void reactivity during a postulated loss-of-coolant accident.

This paper first provides a brief summary of the key model enhancements to the ELESTRES code currently being implemented. Then, the paper describes the verification and validation activities that are being performed in accordance with the AECL SQA program. The paper also discusses interim ELESTRES verification and validation results.

3. QUALITY ASSURANCE

Qualification of the ELESTRES code to model high burnup fuel performance under normal reactor operating conditions, operation at higher coolant pressures and temperatures, and to model $(\text{U,Dy})\text{O}_2$ fuel will be established in accordance with the AECL SQA program and CSA-N286.7-99. The accuracy and adequacy of the models must be demonstrated through verification and validation exercises. The following sections discuss model enhancements, and planned verification and validation activities.

4. MODEL ENHANCEMENTS

Several ELESTRES models were enhanced and/or extended to model the performance of (U,Dy)O₂ fuel, to improve the code's capability to simulate the behaviour of fuel operated to higher burnups, and operation at higher coolant pressures and temperatures than current CANDU fuel. The following key enhancements were made to ELESTRES, based on gap assessment.

4.1 Thermal Conductivity

Irradiation affects the thermal conductivity of the fuel pellet. The ELESTRES-IST [3] thermal conductivity model has been improved to account for the effects of dissolved and precipitated fission products on thermal conductivity. Because the model was not applicable to (U, Dy)O₂ pellets, the thermal conductivity model has been extended to include the effect of Dy on the fuel pellet thermal conductivity, based on measurements of thermal conductivity for (U, Dy)O₂ fuel that cover Dy concentrations up to 13 wt% Dy/Uranium and temperatures up to 1800°C.

4.2 Flux Depression

The heat generation rate within a fuel depends on the distribution of thermal neutron flux and the amount of fissile material within the pellet [2]. The fissile content of the fuel varies as a function of irradiation and the pellet radius because the ²³⁵U is destroyed in the fission process and some ²³⁸U are converted to ²³⁹Pu. The thermal neutron flux also varies as a function of irradiation and the radial distance from the pellet centre. Normally, the thermal neutron flux is higher near the outer surface, and it is lower near the centre of the pellet as the neutrons are either absorbed or used to cause fission. The previous flux depression model had limitations in its applications for smaller diameter fuel, higher burnups [3], and (U, Dy)O₂ fuel. Therefore, the ELESTRES code has been enhanced to include a semi-analytical flux depression model for UO₂ fuel that can be used to simulate the high burnup fuel behaviour and to allow manual input of flux depression data used to simulate (U, Dy)O₂ fuel.

4.3 Fission Gas Release

Fission gases are produced during irradiation inside UO₂ grains. The fission gas atoms diffuse to grain boundaries and precipitate as bubbles on the grain boundaries (i.e., intergranular bubbles). The bubbles grow and interlink as more gas reaches the grain boundary, either by diffusion or during grain-boundary sweeping due to grain growth [2]. The intergranular bubbles can also be destroyed (i.e., the gas atoms within the bubbles are redissolved) whenever fission fragments intersect the bubbles.

By implementation of improved models for diffusivity of fission products in UO₂, intergranular bubble-resolution, and grain boundary gas bubbles critical size before interlinking, the ELESTRES fission gas release calculation has been enhanced. Post-

irradiation examination results of fission gas releases indicate that no significant differences exist between UO_2 and $(\text{U}, \text{Dy})\text{O}_2$ fuels at low powers.

4.4 Densification

Irradiation causes densification due to sintering of the UO_2 pellet during in-reactor operation. The previous empirical densification model has been replaced with a microstructure-dependent densification model to improve the code's prediction capability. The densification model accounts for the dependence of pellet densification on pellet microstructures (e.g., grain sizes and pore size distributions) as well as on temperature and burnup.

4.5 Fuel-Pellet-to-Sheath Contact

CANDU fuel sheaths, designed to be collapsible, normally operate in full contact with the fuel pellets. The collapsible fuel sheath provides good heat transfer and thermal performance. Higher burnup operations, however, can lead to increased gas pressures that may prevent full contact of the fuel sheath. If the internal gas pressure exceeds the coolant pressure, gravity can force the pellet to sit at the bottom of the sheath in a horizontal orientation of CANDU fuel. This means that the pellet now sits eccentric to the sheath, so the radial pellet-to-sheath gap can have a different magnitude at each circumferential locations within the non-contact region. The non-uniform radial pellet-to-sheath gap leads to circumferential variation in pellet-to-sheath gap conductance (i.e., radial heat transfer). A model [5] to account for such local circumferential variation in heat transfer has been added into the ELESTRES code to enhance its capability to simulate non-uniform circumferential heat transfer expected in high burnup fuel.

4.6 Sheath Oxidation

Waterside sheath oxidation layer buildup is expected under high burnup and high temperature operations. The oxide layer buildup on the surface of the fuel sheath impedes the transfer of heat from the pellet to the coolant. This results in increases in temperatures of the fuel sheath and the fuel pellet. A sheath oxidation model has been implemented in the ELESTRES code to assess the effect of sheath oxidation on high burnup fuel performance.

4.7 Additional Features

As noted, to simulate $(\text{U}, \text{Dy})\text{O}_2$ fuel, the ELESTRES code was modified by extending its pellet thermal conductivity model to include the effect of dysprosium (Dy) and by allowing manual input of flux depression data for $(\text{U}, \text{Dy})\text{O}_2$ fuel. Other $(\text{U}, \text{Dy})\text{O}_2$ fuel phenomena such as thermal expansion, material properties, pellet microstructure change, pellet densification, fission product swelling, pellet cracking, and fission gas

atom diffusivity are assumed to be similar with UO_2 fuel, based on LVRF irradiations in the NRU reactor at the Chalk River Laboratories. Additional changes to the ELESTRES code include a new input option to facilitate the Best Estimate Analysis Uncertainty (BEAU) methodology, and to allow users to input the fuel pellet finite element mesh data generated externally by using commercially available codes.

5. VERIFICATION

Verification of the ELESTRES code was performed to ensure that the program functions as designed and that its program logic and coding of mathematical expressions are free of errors. The verification exercises were conducted by following a verification plan that was prepared in accordance with the AECL SQA program and CSA-N286.7-99. The verification exercises consisted of six methods: static testing, dynamic testing, line-by-line inspection, unit testing, detailed module testing, and stress testing. The verification methods are briefly described in the following sections.

5.1 Static Testing

Static testing (or static analysis) is the process of analysing a set of source code files for potential errors without executing the code. A commercial program, plusFORT, was used to perform the static analysis. Static testing uncovered no findings that had any significant impact on the calculated results, code functionality, and performance of the ELESTRES code.

5.2 Dynamic Testing

Dynamic testing (or coverage analysis) was performed to assess the percent of the source code that was exercised by a set of test cases and to uncover any potential remaining defects and inconsistencies in the code. The plusFORT program was used to analyse the source code. All major parts of the code segments were executed successfully by the test cases and dynamic testing uncovered no defects in the code.

5.3 Line-by-Line Inspection

Line-by-line inspection involves a visual inspection of the code to demonstrate that the software implementation of the conceptual models is free of errors. The line-by-line inspections of the modified routines confirmed that the coding is consistent with the theoretical description and conceptual model design.

5.4 Unit Testing

The calculations and logic of the modified part were examined in detail to confirm that it functions as intended. Unit testing uncovered no major errors that have impact on code functionality and performance.

5.5 Detailed Module Testing

By using ELESTRES standard test cases, covering different fuel designs and power histories, the impact of the newly implemented models was assessed. The assessment confirmed that the results have no discontinuities, follow expected trends, and are consistent with the changes implemented in the code.

5.6 Stress Testing

The responses of key output parameters such as internal gas pressure, pellet centreline temperature, and sheath strains were monitored for slight changes in values of diametral clearance. Thousands of ELESTRES test cases runs were executed. The stress testing confirmed that there are no undue oscillations of calculated values and that the trends of the calculated values are qualitatively consistent with expectations from fuel performance experts.

6. VALIDATION

6.1 Key Output Parameters and Validation Data

The Technical Basis Document (TBD) provides a foundation for the safety analysis computer program validation process and it includes a complete list of disciplines and corresponding phenomena. The calculations performed in the ELESTRES code cover two disciplines defined in the TBD: Fuel and fuel Channel thermal-mechanical behaviour (FC), and Fission Product Release and transport (FPR). These disciplines are represented by primary phenomena such as fission and decay heating, distribution of heat in fuel, pellet-to-sheath heat transfer, fission gas diffusion, grain boundary sweeping and grain growth, grain boundary coalescence and tunnel formation, fuel cracking, gap retention of fission gas, sheath deformation, and fuel deformation. These are covered by three key output parameters of the code: fuel temperature, fission product release, and fuel deformation. Table 1 and Table 2 show how the key output parameters are linked to the primary phenomena identified in the Validation Matrices (VM).

Validation data from 172 CANDU irradiations were selected to cover the primary phenomena of fuel behaviour that are important for safety assessments. The ELESTRES validation exercises included comparisons against measurements and also comparisons against six analytical solutions, and the results of inter-code comparisons with the FEAT (Finite Element Analysis for Temperature) computer code [6], which was independently qualified. Table 3 and Table 4 show the ranges of key experimental parameters and measurements in the database, respectively.

6.2 Validation Exercises

A formal validation plan was prepared in accordance with the AECL SQA program and CSA-N286.7-99, identifying key output parameters to be validated, validation methods, data set selection, and planned validation exercises. The validation exercises determine the capability and limits of the code and its conceptual models to simulate the required phenomena. The interim results of the validation exercises, which cover the extended range of burnups, for key ELESTRES output parameters are summarized in the following sections.

6.2.1 Fuel Temperature

- The ELESTRES fuel sheath and fuel pellet centreline temperature results showed excellent agreement (Figure 1) with the results from the FEAT code [6] and analytical solutions.
- The ELESTRES fuel sheath temperature predictions were compared with 270 experimental data points from 275°C to 300°C at various burnups. ELESTRES predictions followed experimental trends, and very good agreement was obtained between predictions and measurements (Figure 2).
- The ELESTRES fuel pellet centreline temperature predictions were compared with 278 experimental data points from 750°C to 1500°C at various burnups. ELESTRES predictions were consistent with measurements and captured the measured temperature trends with burnup and power accurately. The mean error (the average difference between prediction and measurement) of the code calculations with respect to measurements was 1°C and the standard deviation was calculated to be 18°C (Figure 3). The prediction error is close to the measurement uncertainty.

6.2.2 Fission Product Release

- Good agreement was obtained between ELESTRES fission gas release calculations and 158 measurements, to a maximum fuel burnup of about 900 MW·h/kg U (Figure 4). The mean error and the standard deviation between calculations and measurements were -2 ml and 12 ml, respectively. On average, the code under-predicted the fission gas release by 10% compared to measurements.

6.2.3 Fuel Deformation

- Figure 5 shows comparisons between ELESTRES sheath strain calculations and 186 strain measurements at the fuel pellet interfaces and at the fuel pellet mid-plane locations. The mean error and the standard deviation between calculations and measurements were -0.1 % and 0.4 %, respectively.

7. CONCLUSIONS

Qualification of the ELESTRES code for high burnup fuel application was planned and implemented in accordance with the AECL SQA program and CSA-N286.7-99. A number of model enhancements and extensions were performed, including a semi-mechanistic flux depression model that is applicable to extended burnup application, a microstructure-dependent fuel pellet densification model that accounts for grain size and pore size distributions, and thermal properties models applicable for (U, Dy)O₂ fuel up to 13% of dysprosium content. The enhancements were extensively verified. Code validation is currently underway. Preliminary validation exercise results showed good agreement between predictions and data from 172 irradiations and 6 independent analytical results. ELESTRES temperature predictions were consistent with measurements and captured the measured trends with burnup and power accurately. The validation exercises also established that the ELESTRES code and its conceptual models are capable of simulating the required fuel phenomena as listed in the validation plan of the code (Table 1).

8. REFERENCES

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Table 1 REQUIRED FUEL PRIMARY PHENOMENA FOR ELESTRES VALIDATION

Phenomena Number *	Phenomena
FC1	Fission and decay heating
FC2	Diffusion of heat in fuel
FC3	Fuel-to-sheath heat transfer
**FC5	Fission gas release to gap and internal pressurization
FC6	Sheath deformation
FC8	Fuel (pellet) deformation
FPR2	Diffusion of fission products
FPR3	Grain boundary sweeping and grain growth
FPR4	Grain boundary coalescence and tunnel interlinkage
FPR6	Fuel cracking (thermal)

*FC number: Identification used in the Validation Matrix for Fuel & Fuel Channel.

*FPR number: Identification used in the Validation Matrix for Fission gas release.

**FC5 is represented in detail by the phenomena of FPR2, FPR3, FPR4, and FPR6.

Table 2 ELESTRES KEY OUTPUT PARAMETERS AND FUEL PHENOMENA

Key Output Parameters	Related Phenomena	
	Output Parameters	Primary Phenomena
Fuel temperature	Sheath temperature	– Fission and decay heating (FC1)
	Pellet centreline temperature	– Diffusion of heat in fuel (FC2) – Fuel-to-sheath heat transfer (FC3)
Fission product release	Fission gas release	– Fission gas release to gap and internal pressurization (FC5)
	Internal gas pressure	– Diffusion (FPR2) – Grain boundary sweeping (FPR3) – Grain boundary coalescence and tunnel interlinkage (FPR4) – Fuel cracking (FPR6)
Fuel deformation	Sheath strain	– Fuel deformation (FC6)

		– Pellet deformation (FC8)
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Table 3 RANGE OF KEY EXPERIMENTAL PARAMETERS IN DATABASE

Experimental Parameter	Range
Peak power	Up to 75 kW/m
Burnup	Up to 900 MW·h/kg U (37 MWd/kg U)
Fuel enrichment	0.7 to 3.3 U-235 wt. % in total U

Table 4 EXPERIMENTAL RANGE

Key Output Parameters	Experimental Range
Fuel temperature	– Sheath temperature: 275°C to 300°C – Pellet centreline temperature: 750°C to 1500°C
Fission product release	– Volume of fission gas release: up to 150 ml (40%)
Fuel deformation	– Mid-plane sheath strain: -0.3% to 1.9% – Ridge sheath strain: -0.2% to 1.4%

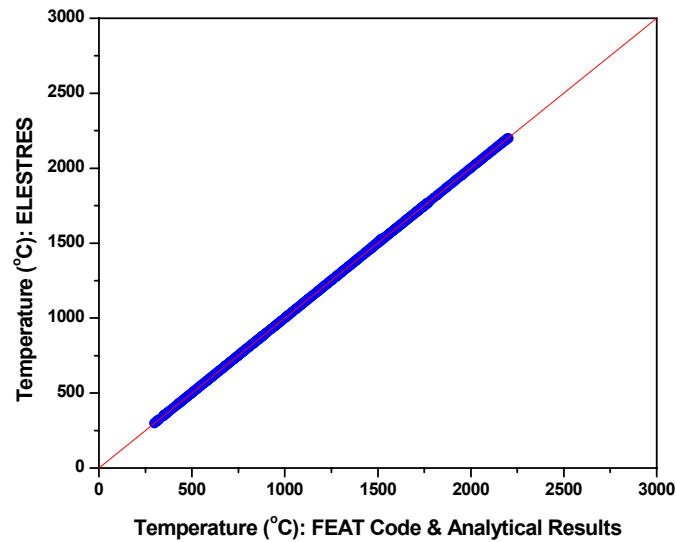


Figure 1 FUEL TEMPERATURE COMPARISONS BETWEEN ELESTRES, FEAT, AND ANALYTICAL RESULTS

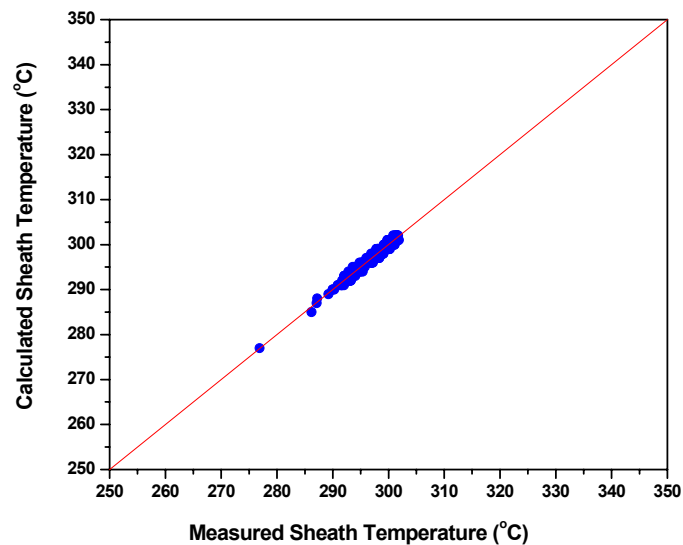


Figure 2 COMPARISON BETWEEN ELESTRES CALCULATION AND MEASUREMENT OF FUEL SHEATH TEMPERATURE

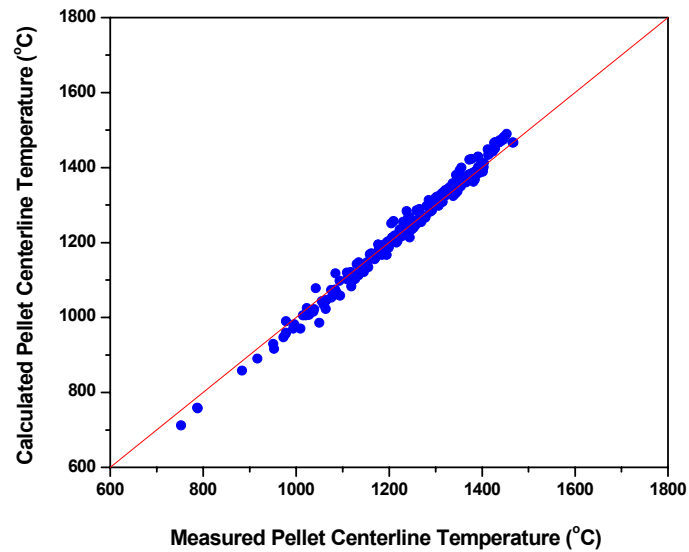


Figure 3 COMPARISON BETWEEN ELESTRES CALCULATION AND MEASUREMENT OF FUEL PELLET CENTRELINE TEMPERATURE

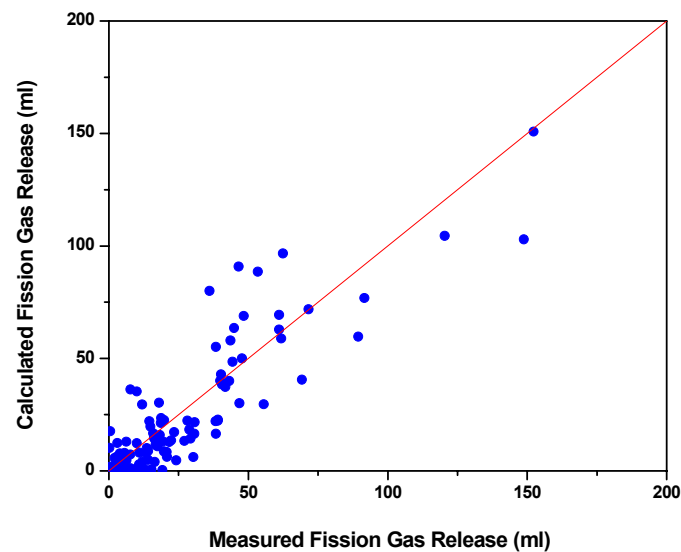


Figure 4 COMPARISONS BETWEEN ELESTRES CALCULATION AND MEASUREMENT OF FISSION GAS RELEASE

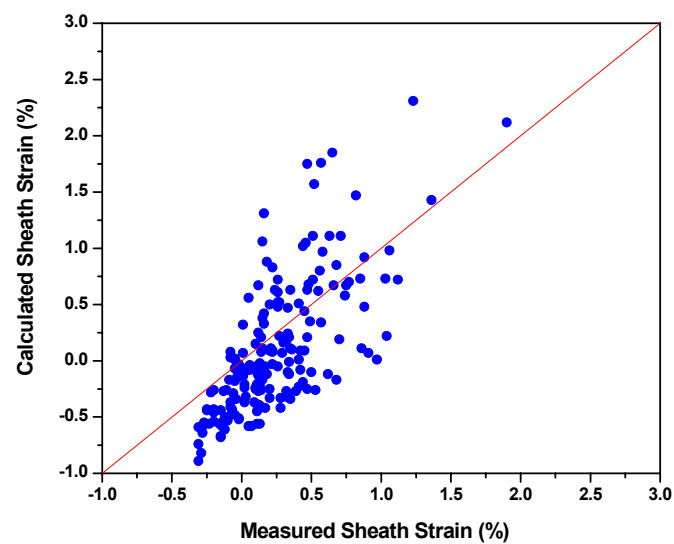


Figure 5 COMPARISONS BETWEEN ELESTRES CALCULATION AND MEASUREMENT OF SHEATH STRAIN