PROGRESS IN QUALIFYING ELESTRES-IST 1.0 CODE: VERIFICATION AND INTERIM RESULTS OF VALIDATION

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ABSTRACT

The computer code ELESTRES-IST 1.0 has been selected as the industry standard tool (IST) for simulation of CANDU® fuel behaviour under normal operating conditions (NOC). As part of formal qualification of the code, ELESTRES has been independently verified and validated according to the Canadian nuclear industry's Quality Assurance Program. The interim results of the verification and validation of the code are described.

1. INTRODUCTION

The ELESTRES code [1] models the thermal, microstructural and mechanical behaviours of a CANDU fuel element under normal operating conditions (NOC). The code is used in reactor safety analyses to quantify pre-accident conditions of fuel elements such as fission gas release, stored thermal energy and fuel deformation. The code is also used in design assessments of CANDU fuel elements.

The ELESTRES-IST 1.0 code has been selected as the industry standard tool (IST) for simulation of CANDU fuel behaviour under NOC. This version of the code contains 11 enhancements over the previous reference version. This functionality of the code was frozen in fall of 1998. Subsequently, the code has been verified and validated according to the requirements of the Canadian nuclear industry's Quality Assurance Program, which is based on standard N286.7 of Canadian Standards Association.

This paper focuses on the interim results of verification activities and validation exercises. In addition, a brief background is given of the recent enhancements of the code.

2. RANGE OF APPLICABILITY

The following are the applicable ranges of the ELESTRES-IST code:

- CANDU fuel element under normal operating conditions, i.e., nominal system pressure, wet sheath, and nominal powers and temperatures;
- stoichiometric UO_2;
- pellet diameters of 12.15 to 19.5 mm, pellet enrichments of 0.71 to 6.0 wt.% U-235, and fuel burnups to 480 MWh/kg U, to be consistent with the look-up table for flux depression in UO_2 pellet;

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- peak rating less than 83 kW/m, to prevent UO_2 melting;
- sheath temperature about 300°C, to be consistent with sheath creep correlation;
- collapsible sheaths.

The code has been benchmarked with 20 selected irradiations from the Irradiated Fuel Database.

3. ENHANCED FEATURES OF CODE FUNCTIONALITY

3.1. Thermal Conductivity. The existing correlation for calculating the thermal conductivity of UO_2 fuel was improved to take into account burnup effects.

3.2. Enhanced Fission Gas Release Models. The model for fission gas release has been enhanced in the areas of grain boundary sharing, diffusion of new gas, grain boundary sweeping, and hydrostatic stress.

3.3. Enhanced Numeric Stability in Sheath Creep. The sheath creep equations are now solved with a fully explicit method. This has eliminated occasional numeric instabilities that were sometimes encountered in the previous version's fully implicit scheme.

3.4. Incremental Densification Incremental densification is now calculated by capturing the effects of instantaneous changes in pellet temperature at each burnup step. This eliminates inconsistencies in densification between the end of the previous burnup step and the start of the current burnup step.

3.5. Convergent Finite Element Mesh

Increased Nodalization in Finite Element mesh. The convergence of the spatial solution is now obtained to a smaller tolerance. This is achieved by using a finer finite element mesh that allows up to 30 radial nodes and 45 axial nodes (as opposed to 8 and 14 in the previous version of the code).

Large Chamfers. The finite-element nodalization of the pellet now permits modelling larger chamfers, by adjusting the number of axial nodes.

3.6. Streamlined Output. To give users easier and more comprehensive understanding of calculation results, the code output is now arranged in a more streamlined manner with output tables now collecting similar and closely related parameters. Also, convenient links are now provided to a graphical package such as Excel.

3.7. Application of Software QA Tools. The code has been modified to reflect findings of software QA tools such as SPAG, QA Fortran and plusFORT. Thus, the code now contains significantly more comment cards to explain the code's logic. Also, each subroutine now contains a list of key variables.

4. VERIFICATION

Extensive verification has been performed for the frozen version of the code. It has been conducted by an independent organization (Ontario Power Generation Incorporated) that was not involved in code development. The verification activities have been divided into five parts: static testing, dynamic testing, line-by-line inspection, unit testing, and stress testing. The main results are described below.

4.1. Static Testing. Static testing is the process of analyzing a set of source code files without executing by means of a set of CASE (Computer Aided Software Engineering) tools. A total of 4 static analysis CASE tools were used: FORCHECK, FLINT, HINDSIGHT and SPAG/GXCHK. Static testing uncovered no significant defects in the ELESTRES-IST code. Most of the findings relate to ways the software could be marginally improved from a software engineering perspective, such as the definition of common blocks, the change of a subprogram, etc. None of these would have any impact on calculated results.

The static tests provided a total of 116 messages. Of these, 67 were judged to be important, and were addressed via code modifications. The remainder, 49, were judged to be trivial and ignored. The independent verifier accepted these resolutions.

4.2. Integrated Code Testing (Dynamic Testing). Dynamic testing has been performed to assess what fraction of the code is executed by a standardized set of 37 test cases. The SPAG/CVRANAL tool and HINDSIGHT were used. Neglecting some guard code that would trap input error conditions, over 90% of the code segments were executed by the 37 test cases. Each unexercised code segment was examined and reported.

Nine messages reported in dynamic testing were all resolved by code modifications.

4.3. Line-by-Line Inspection. Quality metrics and criteria were established for line-by-line inspection, and formally documented in a Verification Plan. Line-by-line inspection began with a ranking of each subprogram on the basis of the complexity and the importance of the algorithm and the theory. Then, 36 highest-ranked subprograms out of total 108 subprograms were visually inspected for adherence to the list of quality metrics and the criteria outlined in the Verification Plan. Following visual inspection, the arithmetic expressions and constants used in each subprogram were compared with the description in the ELESTRES-IST Theory Manual. Equations or constants that could not be easily compared to the Theory Manual due to their form were verified through unit testing.

The deviations were classified as Major, Potentially Major, and Minor. Any possibility or potential to affect calculation results was classified as either of Major or Potentially Major deviation. A deviation was called Minor when the condition was related more to the quality of the source code than the quality of the tool's output. Sixty-three deviations were reported by the verifiers; 2 were classified as Major, 8 classified as Potentially Major, and 53 were classified as Minor.

Both the Major deviations, and all 8 Potentially Major deviations, were resolved via code modifications. Fifteen of the Minor deviations were also resolved via code modifications. The remaining Minor deviations were judged to be trivial, and an informed decision was made that they required no immediate action.

4.4. Unit Testing. Sixteen units, including 34 subprograms, were tested as independent units. Most of these subprograms were routines that were highly ranked based on criticality and complexity. Some additional subprograms were added to these, based on lack of segment coverage discovered during dynamic testing or due to unclear construction found during line-by-line inspection. The verifiers reported thirteen findings. In general, the findings were of minor significance to the overall calculation of ELESTRES-IST; nevertheless, all thirteen findings were resolved via code modifications.

4.5. Stress Testing. The ELESTRES-IST code was compiled and tested for 53 test cases and 5 detailed impact assessment cases. Further, three thousand additional runs were also made as part of stress and regression testing. All test cases were completed successfully, and test results were compared with the test results of the previous beta version.

The previous beta version of the code showed some discontinuities in the code that were not physical. The root causes were investigated, located, and removed. The final IST 1.0 version of the code shows no discontinuities, as illustrated in Figure 1.

4.6. Resolution of Verification Findings. A total of 212 messages were generated; 12 Major and 200 Minor. All the major findings, and most of the minor findings, were resolved via code modifications. Resolution of cosmetic and inconsequential messages was deferred to a later date. In addition, 34 suggestions from users were implemented.

5. VALIDATION

5.1. Validation Data. Validation data were selected to cover 9 primary phenomena of fuel behaviour that are important for safety assessments.

These phenomena were derived through a review of the Technical Basis Document (TBD) for safety analyses, and the Validation Matrices (VM) for Fuel and Fuel Channel and for Fission-gas Release. The phenomena include 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 shows how the key output parameters are linked to the primary phenomena identified in the Validation Matrices.

The validation exercises included comparisons against 110 different experiments and also comparisons against 6 independent analytical/numerical solutions, for a total of 116 different test cases. Table 2 shows the ranges of key experimental parameters in the database, and Table 3 shows experimental range versus expected range.

5.2. Validation Exercises. A formal validation plan was prepared ahead of time, identifying key output parameters to be validated, validation methods, data set selection, and planned validation exercises. The key results of the validation exercises are summarized statistically in Table 4.

5.2.1. Fuel Temperature.

- For the six analytical validation cases of fuel temperature, the calculations of the ELESTRES-IST code showed perfect agreement with the analytical solutions and with another independent code. These results confirm that the ELESTRES-IST code has correctly solved the fundamental equation for conduction of heat through the fuel element. (Figure 2).
- The ELESTRES-IST code calculations of sheath temperature were consistent with 270 measurements in the range of 275 to 310°C at various burnups. The code followed all trends measured in the experiment. A nearly perfect match was obtained between calculations and measurements (Figure 3).
- The ELESTRES-IST fuel pellet centre-line temperature calculations were consistent with 278 experimental measurements in the range of 750 to 1500°C and captured the measured temperature trends with burnup and power very well. Overall, the ELESTRES-IST calculations were lower, on average, by 4% in comparison to these measurements (Figure 4).

5.2.2. Fission Product Release

- ELESTRES-IST code calculations of fission gas release were consistent with experimental measurements: the code underpredicted the release by 6% on average. No statistically significant bias was detected (Figure 5).
- ELESTRES-IST code calculations of internal gas pressure were consistent with experimental data measured: the code underpredicted the pressure by 9% on average, but the prediction error of 9% is within the measurement error of ±10% (Figure 6).
- Most scatter in the measured gas release and gas pressure were explained by taking into account the uncertainty of ±10% in power (Figure 7).
- ELESTRE-IST code calculations of gas diffusion, free voidage (Figure 8) and pellet grain-growth/ microstructure changes (Figure 9) were consistent with experimental measurements.

5.2.3. Sheath Strain.

- ELESTRES-IST code calculations of sheath strain at pellet mid-plane were consistent with 58 experimental data: the code slightly overpredicted the sheath strain by 4%, on average, over the values of a perfect match (Figure 10).
- ELESTRES-IST code calculations of sheath strain at ridge were consistent with 41 experimental data: the code calculations were very close to a perfect match on average (Figure 10).

6. CONCLUSIONS

The ELESTRES-IST 1.0 code has been selected as the industry standard tool for simulation of CANDU fuel behaviour under normal operating conditions . The code contains 11 enhancements over the previous reference version The code has been extensively verified and validated per the Canadian nuclear industry's Quality Assurance Program. All significant verification findings have been addressed. Validations show that the code exhibits a good match with data from 110 irradiation experiments and 6 independent analytical results.

7. REFERENCES

[1] TAYAL , M., "Modelling CANDU Fuel under Normal Operating Conditions, ELESTRES Code Description", AECL, Report AECL-9331, 1987 February.

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Table 1 ELESTRES-IST Key Output Parameters and Related Fuel Phenomena

Key Output Parameters	Related Phenomena	
	Output Parameters	Intermediate Parameters
Fuel temperature	Sheath temperature Pellet centreline temperature	Fission and decay heating (FC1*) Diffusion of heat in fuel (FC2) Fuel-to-sheath heat transfer (FC3)
Fission product release	Fission gas release Internal gas pressure	Fission gas release to gap and internal pressurization (FC5) - Diffusion (FPR**2) - Grain boundary sweeping (FPR3) - Grain boundary coalescence and tunnel interlinkage (FPR4) - Fuel cracking (FPR6)
Fuel deformation	Sheath strain	Sheath deformation (FC6) Pellet deformation (FC7)

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

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

Table 2 Range of Key Experimental Parameters in Database

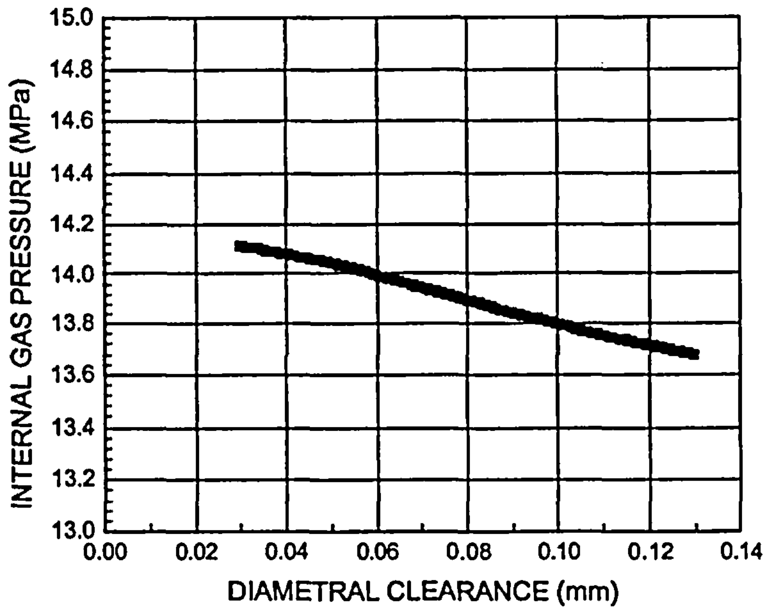
Experimental Parameter	Range
Peak power	Up to 76 kW/m
Burnup	Up to 469 MWh/kgU
Fuel enrichment	0.71 ~ 3.3 U-235 wt. %
Pellet diameter	12.15 ~ 19.0 mm
Coolant temperature	Up to 303 °C (Single phase)
Coolant pressure	Up to 10.7 MPa (Single phase)

Table 3 Experimental Range

Key Output Parameter	Output Parameter	Experimental Range
Temperature	- Pellet centreline temperature - Sheath temperature	• Pellet centreline temperature; - Direct measurement: 750-1500°C - Indirect measurement: up to 2450°C • Sheath temperature: - Direct measurement: 270-310°C. - Indirect measurement: up to 350°C.
Fission product release	- Volume of fission gas release - Internal gas pressure	• Volume of fission gas release: up to 130 cm^3 • Gas pressure: up to 8.0 MPa.
Fuel deformation	- Hoop strain in the sheath	• Mid-plane sheath strain: -0.31 to 0.65% Ridge sheath strain: -0.15 to 1.23%

Table 4 Statistical Analysis Results

	Fuel Temperature (°C)		Fission Product Release		Sheath Strain (%)	
	Pellet center	Sheath surface	Gas volume (ml)	Gas pressure (MPa)	Mid-plane	Ridge
No. of data	278	270	94	311	58	41
No.of irradiations	1	1	94	4	58	41
Slope of Linear regression, y=m x	0.96	1.0	0.94	0.91	1.04	1.0



(Note: This figure represents approximately 3000 runs of ELESTRES-IST.)

Figure 1 Example of a Stress Test

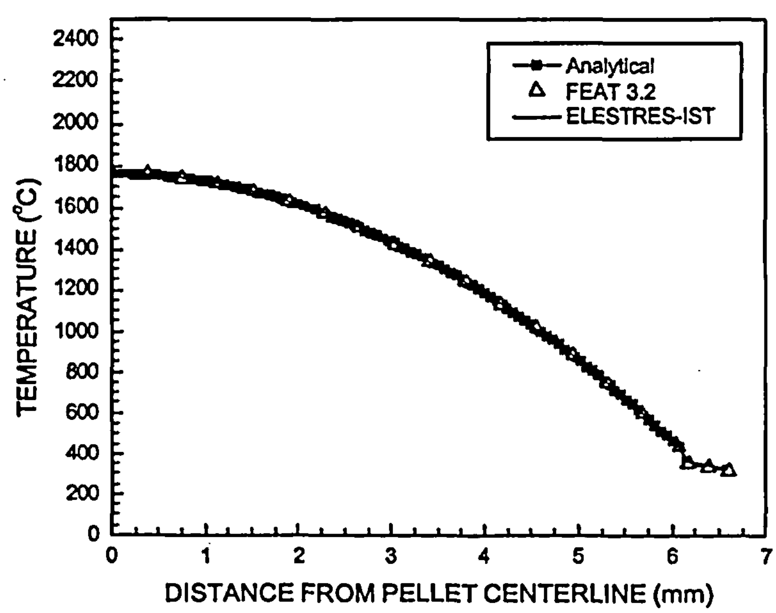


Figure 2 Pellet Centerline Temperature: Comparison with Two Independent Solutions

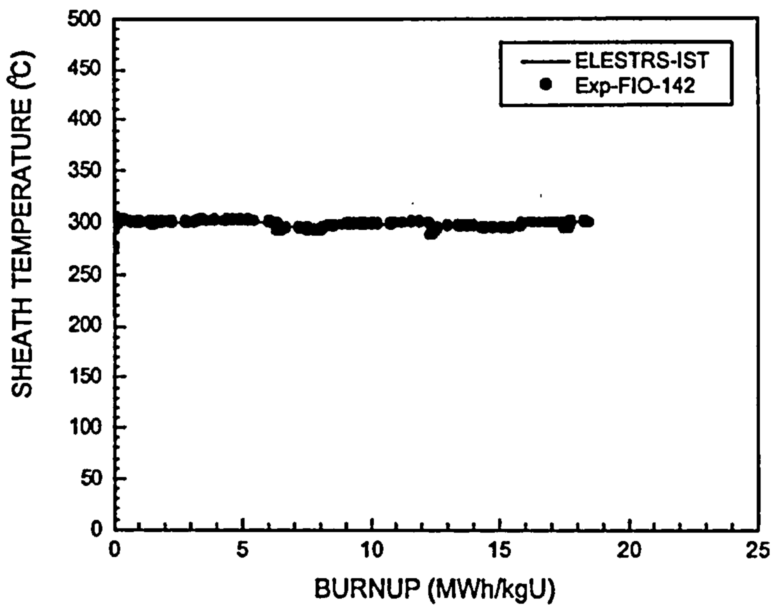


Figure 3 Sheath Temperature: Comparison with Measurements from Irradiation FIO-142

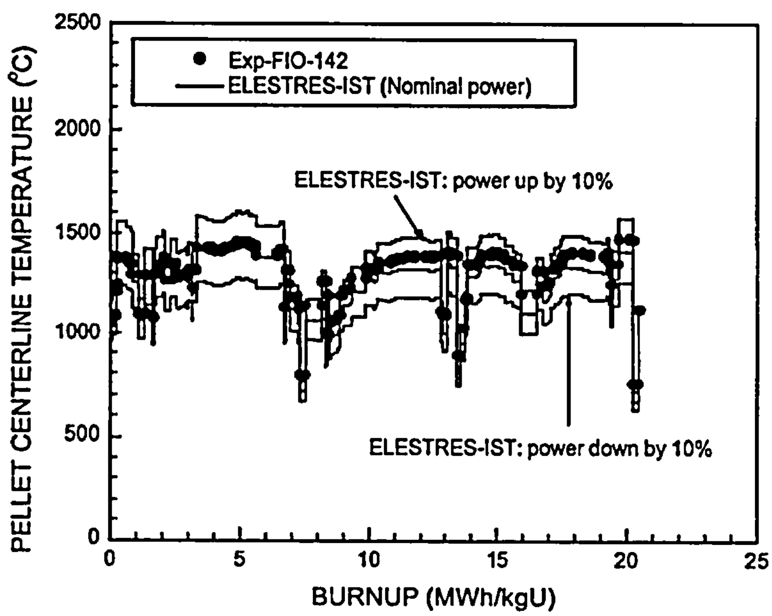


Figure 4 Pellet Centerline Temperature: Comparison with Measurements from Irradiation FIO-142

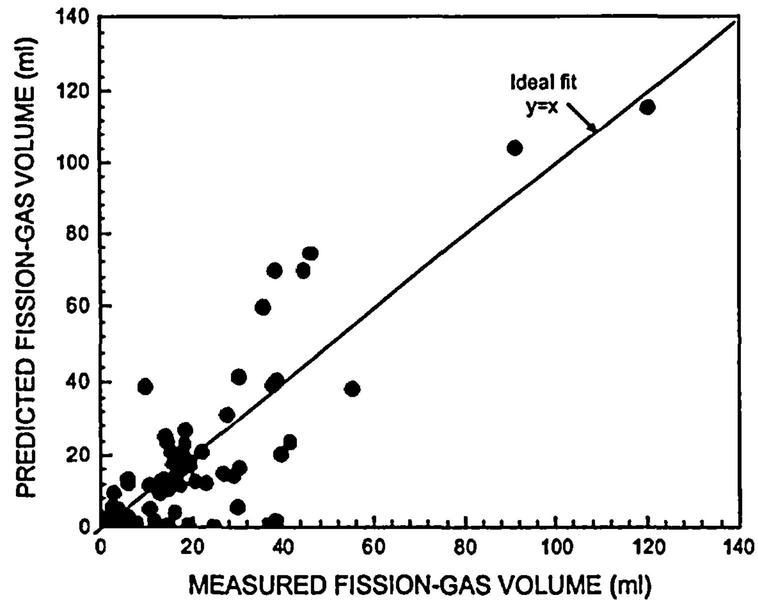


Figure 5 Fission Gas Release: Comparison with All Measurements

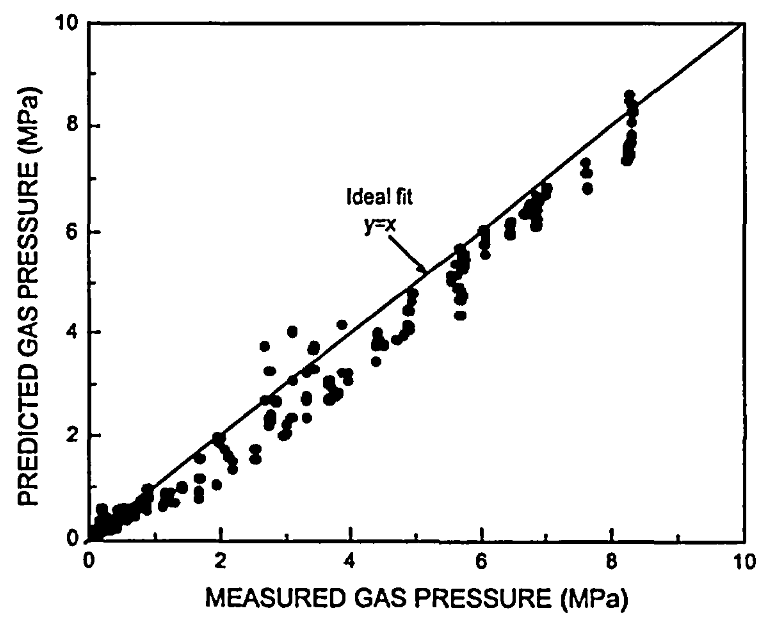


Figure 6 Internal Gas Pressure: Comparison with Measurements from 4 Irradiations (LFX, LFW, ARY, ARZ)

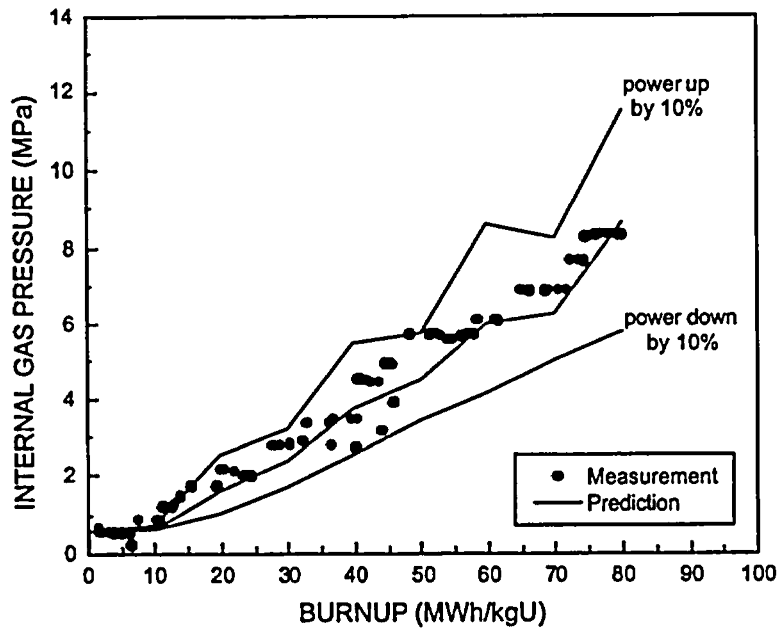


Figure 7 Internal Gas Pressure: Comparison with Measurements from Irradiation LFX, Including the Influence of Power Uncertainty

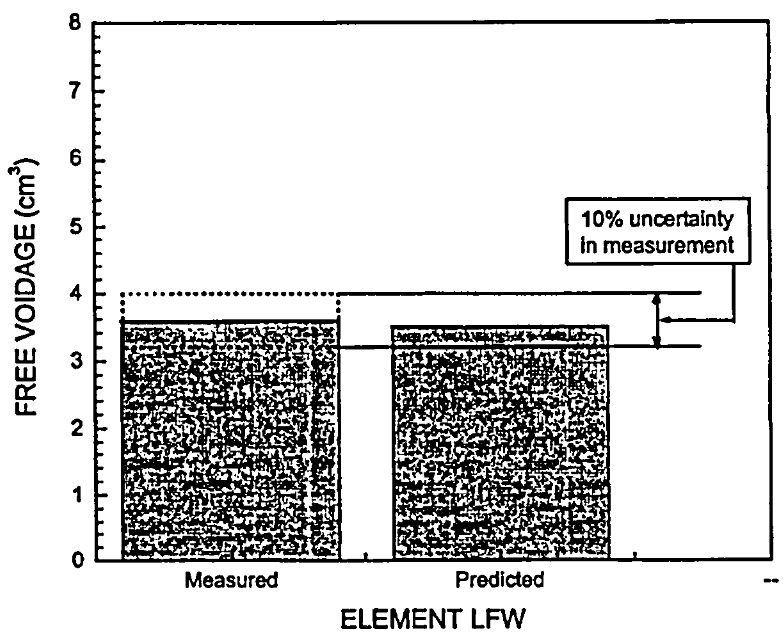


Figure 8 Free Voidage: Comparison with Measurement from Irradiation LFX

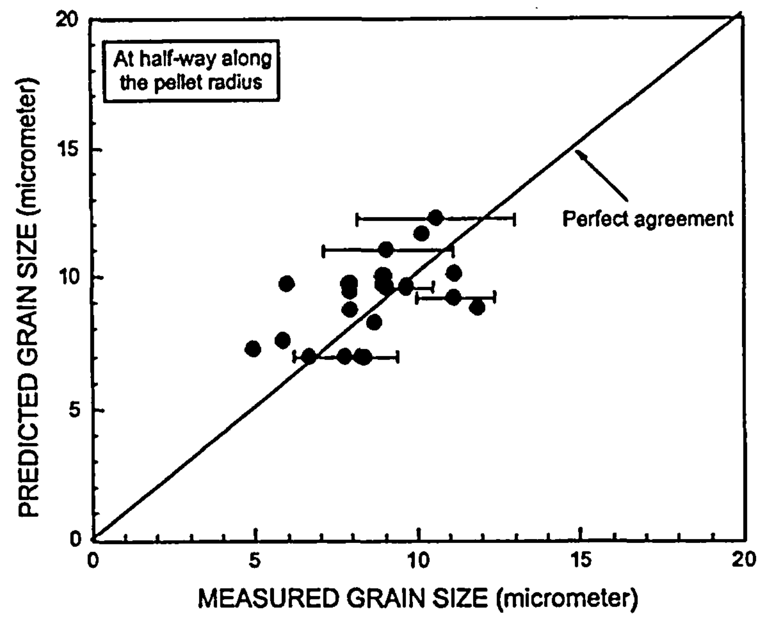
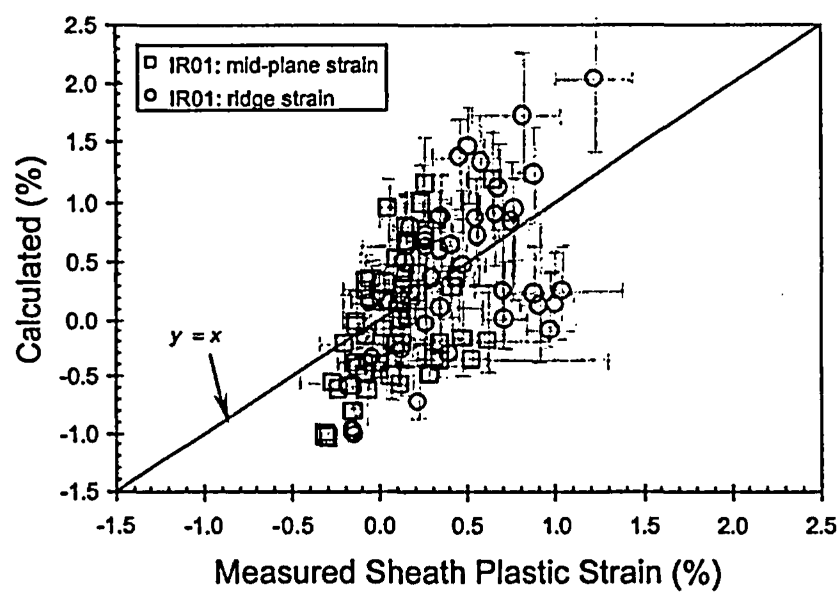


Figure 9 Pellet Grain Growth: Comparison with Measurements for All Data



(Note: Horizontal error bars represents scatter in measurements, and vertical error bars represent ±10% variation in power.)

Figure 10 Sheath Strains: Comparison with Measurements for All Data