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Authors:	M. L. Williams R. J. Ellis K. T. Clarno F. C. Difilippo J. C. Gehin
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OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831-6170
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M. L. Williams, R. J. Ellis, K. T. Clarno, F. C. Difilippo, J. C. Gehin
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6170

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Oak Ridge National Laboratory

P.O. Box 2008

Oak Ridge, TN 37831-6170

I. INTRODUCTION

As described in of the Statement of Work for the NRC RES funded project entitled, "ACR-Lattice Physics Models, Data, and Validation," (NRC JCN Y6846) ORNL will assess the bias and uncertainty in the coolant void reactivity (CVR) for the Advanced CANDU Reactor, ACR-700. A preliminary program plan to accomplish these objectives was provided to the NRC in a letter report entitled "Application of Sensitivity Analysis to Quantify the Bias and Uncertainty in Calculated ACR-700 CVR" (ORNL/NRC/LTR-04/14). The recommended approach is as follows: 1) Development, verification, and validation of the lattice physics methods to be used for the sensitivity/uncertainty (S/U) analysis and for the few-group homogenized cross sections for transient analysis; 2) Development of the S/U methodology for the CVR as a response; 3) Evaluation of AECL experimental program for the ACR-700; and 4) Nuclear data, including covariance data, for the ACR-700 CVR bias assessment.

ORNL/NRC/LTR-04/14 provides an overview of the work to be performed, the program objectives and a discussion of the program plan. Work is proceeding on the plan described in that report. This letter report provides an update to ORNL/NRC/LTR-04/14 to address the need for information to evaluate the applicability and adequacy of the planned test program for the ACR neutronics, and based on that evaluation provide timely identification of any significant gaps in the planned validation database. Additional information is provided on the development of the S/U methods to be used to assess the nuclear data uncertainties and on the development of the lattice physics methods.

In the sections below, the specific needs for experimental data are discussed for the verification and validation of SCALE 5 for ACR analysis, review and assessment of the ACR experimental program. In addition, the need for additional nuclear data is discussed.

II. VERIFICATION AND VALIDATION OF THE SCALE 5 METHODS AND DATA

The SCALE 5 computer system will form the basis for the CVR analysis at ORNL; thus it is important to establish the accuracy of the SCALE calculational methods for ACR-700 analysis. The S/U analysis will be performed using a SCALE calculation sequence that performs lattice physics calculations to obtain self-shielded multigroup cross sections, followed by a 3-D criticality calculation performed with the multigroup Monte Carlo code KENO-Va or KENO-VI. The TRITON sequence will be used to generate few-group cross section parameters for PARCS/TRACE modeling. Validation of the nuclear data libraries, resonance processing and self-shielding methods, and neutron transport methods will be necessary. The general area of SCALE lattice physics validation is to be addressed in detail in the Statement of Work under Task 2 of this NRC project (JCN Y6846), in conjunction with Brookhaven National Laboratory.

An initial assessment of the resonance self-shielding and other lattice physics methods is necessary prior to the S/U analysis and cross section generation analysis, to insure that appropriate techniques are used. An approach for modeling the ACR-700 fuel bundles has been developed at ORNL using the NITAWL approach for ENDF/B-V and CENTRM for ENDF/B-VI libraries. Initial comparisons have been performed with MCNP calculations to verify the results. Additional, preliminary verification will be performed by comparing SCALE results to those obtained by BNL using MCNP/MONTEBURNS, Purdue University using HELIOS, and available AECL results.. A “numerical benchmark” for unvoided and voided bundle models as well as 2x2 configurations has been proposed by Purdue University and will be used for verification by comparing the SCALE 5 KENO V.a and TRITON results to MCNP results obtained using the same basic cross section data. Methods identified as causing an excessive uncertainty will be addressed by modifying the computational or modeling techniques in SCALE.

These verification calculations, however are not sufficient for validation of the SCALE 5 methods and data. Comparisons with experimental data are required for this purpose. The experimental data should be provided by AECL as part of their ACR-700 experimental program, which will be further discussed in Section V.3. Data need includes critical experiments for voided and unvoided configurations for ACR-specific fuel designs including enriched fuel, light-water coolant, and dysprosium pins. In addition, PIE isotopic data are required for the validation of fuel depletion methods. Existing, relevant critical experiment and PIE data can be used immediately for preliminary validation followed later with the ACR-specific data when available.

III. ACR EXPERIMENTAL PROGRAM ASSESSMENT AND REVIEW

A series benchmark experiments will be performed by AECL in the ZED-2 facility to validate the computation methods and nuclear data used for the ACR-700 design. AECL has provided an initial summary of their strategy to support ACR physics issues with ZED-2 experiments [in ACR document 108-123110-440-002 (FFC-RRP-464) Rev.0 from September 2003 entitled "Planned Experiments in ZED-2 in Support of ACR"]. A critique will be performed by ORNL on the AECL plan for their series of proposed ZED-2 experiments. Of particular importance, an assessment will be made to determine if the planned experiments will validate and provide necessary information pertinent to ACR-700 safety-related issues such as checkerboard and full-voiding CVR, and other reactivity temperature effects. During July 2004, a series of meetings on ACR physics issues was held between NRC and its contractors, and AECL, with CNSC also present. ORNL representatives toured the ZED-2 facility. AECL mentioned that a revised ZED-2 experimental program plan, in support of ACR-700, would be distributed soon. The adequacy of the planned ZED-2 experimental program will be examined, and input will be provided on what improvements are needed and which additional experimental configurations would be beneficial.

In order to assess the AECL experimental program in support of the ACR-700 and have data for the verification and validation of the SCALE 5 methods and data, detailed information on the AECL ACR and other experiments is required. AECL must provide the updated experimental program plan for review. This plan should include a comprehensive discussion of all existing and planned ACR-relevant experiments not only including ZED-2, but also those from other facilities such as DCA (Japan), DIMPLE (U.K.), ECO (Italy), and Savannah River. PIE nuclide assays from all relevant fuel irradiations in NRU and operating CANDU reactors are also of interest for the validation of the fuel burnup calculations. Any planned ACR-specific irradiations should also be discussed.

Detailed specifications of each of the existing and proposed experiments are also required with sufficient detail to define 3-D KENO "whole-core" models to allow benchmarking and validation. AECL must also provide necessary technical information on all associated measurements, measurement techniques, and measurement uncertainties. In particular, detailed information on the qualification and use of the zone substitution techniques, and the associated CONIFERS code, in the context of the specific ACR-700 experiments in ZED-2.

In this regard, ORNL could make immediate use of the documents listed in Table 1. These documents and information are requested to assist in the assessment of ZED-2 and ACR-700 nuclear data issues. Recently, ORNL has reviewed the available information for the ZED-2 experiments and began preliminary model development. Of particular importance are the details of the ZEEP booster fuel rods used in some ZED-2 experiments to ensure criticality. Other relevant documents, not listed in Table 4, should also be provided.

A main goal of the ZED-2 experiments is to provide data which can be used to validate the AECL computer codes and tools which will be used for AECL ACR-700 calculations and analyses. For example, experiments that represent checkerboard voiding scenarios (with representative fresh and burned fuel assemblies) will be very important in validating the CVR calculations, since checkerboard situations with possible positive void reactivity consequences were identified during the ACR-700 PIRT panel process. Also, experiments that provide information on the ACR core neutron leakage trends will be very important since leakage is a major component in the overall CVR.

The ORNL S/U codes will be utilized to quantify the similarity of the neutronic environments in the ZED-2 experiments and the actual ACR-700 lattice. S/U methods will also be applied to available measurements from other benchmark facilities to determine their suitability for the ACR-700 validation program. There is an ongoing need for covariance data of nuclides such as Dy, ^{239}Pu, and heavy water that are important to CVR computations for the ACR-700, since S/U methods utilize these data in the experimental analysis.

IV. NUCLEAR DATA

Analysis of the ACR equilibrium core will require nuclear data for numerous nuclides due to the presence of fission products and higher actinides. SCALE nuclear data libraries based on ENDF/B-V are currently available for most materials; however, the SCALE ENDF/B-VI cross section libraries have not been officially released. ORNL has recently began the use of the ENDF/B-VI data libraries for the ACR-700 analysis to provide consistent comparisons with MCNP results. A covariance library based on ENDF/B-V (supplemented by a few additional nuclides) is also available; but the covariance data in both ENDF/B-V and ENDF/B-VI is incomplete. Additional nuclear data and covariances may be available from other sources such as JEF, JENDL, CENDL, and BROND.

A list of nuclides needed for analysis of the ACR-700 equilibrium core is shown in Table 2 (obtained from AECL Assessment Document, "ACR-700 Reactor Physics Design," dated 6/6/2003). The current SCALE nuclear data libraries based on ENDF/B-V have all of the required materials except for ^{238}Np and ^{239}Np, and the two lumped fission products. The lumped fission products will either be ignored or approximated in some reasonable manner. The SCALE ENDF/B-VI multigroup libraries are being finalized, and will be utilized for ACR-700 analysis when available in a short period of time.

The use of S/U methods, described more fully in ORNL/NRC/LTR-04/14, require cross section covariance data to obtain a quantitative assessment of uncertainties resulting from nuclear data. The TSUNAMI S/U methods will be extended to include the CVR as a response so that the nuclear data contributions to the CVR uncertainties can be quantitatively evaluated. In addition, the TSUNAMI S/U methods will be applied to the assessment of the ZED-2 and other experiments to determine their applicability to the ACR-700 design. Despite new measurement and evaluation initiatives, the ENDF/B files have a limited amount of covariance data available for applications. ENDF/B-V has 30 materials with covariance data, while ENDF/B-VI.8 has covariances for 49 materials. Table 3 summarizes the materials for which covariances are available on ENDF, while Tables 4a and 4b show the materials in the multigroup covariance libraries that have been processed for use in the ORNL S/U calculations. The current SCALE covariance data are based on ENDF/B-V supplemented by data obtained from Argonne National Laboratory.

Under direction of the DOE Nuclear Criticality Safety Program, covariance data needs have been identified for high-priority materials in criticality safety applications. As part of this effort ANL, LANL, and ORNL will generate new data for the following nuclides over the next three years:

^{239}Pu, ^{240}Pu, ^{241}Pu, ^{16}O, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{14}N, ^{9}Be, ^{235}U, ^{238}U, ^{55}Mn, ^{19}F, ^{39}K, ^{41}K, B, C, Na, Mg, Ga, Pb, Fe, Ni, Cr, Cu, Ce, Ca, Hf, Er, Th, Nb, Am, Np.

Several important isotopes for the ACR analysis are included in the above list; however, many nuclides shown in Table 2 are missing from this list. Most notable are the dysprosium isotopes, deuterium, and numerous fission products. Also, no covariance data for any thermal scatter laws [S(α, β) data] have ever been generated, so the uncertainties due to the light and heavy water thermal scatter kernels can not be assessed. This may not be a significant effect, but it has never been studied. Sensitivity coefficients for the scatter matrix elements in the thermal range may provide some guidance in this area.

The lack of cross section covariance data must be addressed. Some notable progress has been made in this area. An approximate method to generate covariance data was developed to supplement the more rigorous approach being supported under other programs for some of the important nuclides. It is expected that covariance data will be generated for all materials required in the ACR-700 analysis within the next several months.

V. RECENT PROGRESS AND DEVELOPMENTS

Equations for CVR sensitivity coefficients were obtained using two different approaches: one is based on the "exact perturbation theory" expression for reactivity and requires generalized perturbation theory; the other uses the eigenvalue-difference formulation of reactivity and can be performed using standard eigenvalue perturbation theory. It appears that our initial goals can be accomplished with the latter approach; thus, only minor changes in the TSUNAMI codes will be required. Equations describing computation of the CVR uncertainty have also been obtained, and will be implemented into the Generalized Least-Squares code that computes bias magnitude and uncertainty.

In order to establish the adequacy of multigroup KENO calculations for the S/U analysis, detailed comparisons were made between SCALE and MCNP results for unvoided and voided fuel bundle models. Initial results were based on ENDF/B-V, but ENDF/B-VI libraries processed for SCALE were recently tested against the MCNP results. As result of this analysis, ENDF/B-VI data at an additional temperature were processed and are now being evaluated.

The SCALE lattice-physics techniques were validated by comparing multigroup cross sections with values obtained from MNCP. It was decided that the CENTRM/PMC modules in SCALE should be used to produce problem-dependent 238-group data for 3D KENO calculations of the CVR sensitivity coefficients. CENTRM, which uses discrete ordinates to compute pointwise (PW) spectra for self-shielding calculations, was found to give a better treatment for resonance overlap and interference effects than the NITAWL module in SCALE, and also is needed for use with ENDF/B-VI data. Thus, most of the future S/U analyses will be based on this approach. It was found that CVR results are quite sensitive to the Dancoff values used for self-shielding; therefore Dancoff factors for each fuel ring are obtained from 3D Monte Carlo calculations of the ACR lattice, and are input into the SCALE lattice physics computations. A new technique was developed to utilize Dancoff factors in the CENTRM unit cell calculations. The preliminary CVR results obtained in this manner appear to agree reasonably well with MCNP, and should be adequate to compute forward and adjoint neutron fluxes for the S/U analysis

One unique feature of the ORNL computations of sensitivity coefficients is that "implicit" effects are treated. Implicit effects represent the impact of cross section uncertainties on self-shielding of multigroup data, while explicit effects account for direct effects on the eigenvalue calculation. For example, an uncertainty in the evaluated hydrogen cross section causes an uncertainty in the multigroup hydrogen cross section that directly impacts the KENO eigenvalue calculation by perturbing neutron moderation, etc. This is the explicit effect. However, an uncertainty in the H cross section also impacts the self-shielding of ^{238}U multigroup cross sections, for example, due to its impact on the Dancoff factor. The associated uncertainty in the ^{238}U multigroup cross section caused by hydrogen data also implicitly affects the eigenvalue calculations. The current TSUNAMI codes use NITAWL to determine the implicit sensitivity coefficient; however, as previously discussed, the CENTRM module will be used for future ACR calculations. Several potential approaches for using CENTRM to compute implicit sensitivity coefficients have been proposed and are currently being evaluated.

Table 1. Information Request for Assessment of Experimental Program

1. R.J. Ellis, "Redistribution of Technical Note (Reactor Technology Branch) RTB TN 010: MCNP Analysis of 37 Element UO2 Bundle Core Measurements in ZED 2", RRP 97 159, 1997 October 10. (In addition, the associated MCNP input file by R.J. Ellis for ZED-2 is requested.)

2. R.J. Ellis, "MCNP Analyses of 37 Element UO2 Bundle Core Measurements in ZED 2", RTB TN 010, 1994 September.

3. J.V. Donnelly, R.J. Ellis, and P.J. Laughton, "Effect of Changes in 239Pu between ENDF/B V and ENDF/B VI on CANDU Coolant Void Reactivity", Memorandum to P.G. Boczar, 1995 November 16.

4. J.V. Donnelly and R.J. Ellis, "Monte Carlo Analysis of ZED 2 Substitution Measurements of Low Void Reactivity CANDU Fuel", RTB TN 038, 1995 February.

5. R.J. Ellis, "New Measurements of Fuel Positions in ZED 2", Reactor Technology Branch memorandum RJE 94 098, 1994 April 12.
6. M.B. Zeller, "Recommended Enrichment of SEU for Proposed ZED-2 Physics Experiments in Support of NG CANDU", FFC-RRP-393, 2001 October.

7. M.B. Zeller, A. Celli, and G.P. McPhee, "Lattice Physics Measurements Using LVRF in CANDU-Type Channels Performed in ZED-2", Research Company Report, RC-1500, 1995 November.

8. F.N. McDonnell and A. Okazaki, "Bucklings of Heavy Water Moderated Lattices of ZEEP Rods", AECL-3998, 1971 September.

9. M.B. Zeller, et al, "Room-Temperature Substitution Measurements using Simulated CANDU Mid-Burnup Fuel in CANDU-Type Channels", FFC-RRP-094, 1998 March.

10. R.E. Green and C.W. Colpitts, "CANDU-BLW Experiments in ZED-2 Part III: Buckling and Loss of Coolant Experiments", AECL-2961, 1967 May.

11. R.S. Davis, A. Celli, J. Griffiths, R.T. Jones, D.C. McElroy, M.B. Zeller, "Validation of the Chalk River Method of Analyzing Substitution Experiments by Comparison with Full-Core Measurements Volume I: Method", FFC-RRP-97/COG-98-83, Volume I, 1999 April.

12. R.S. Davis, A. Celli, J. Griffiths, R.T. Jones, D.C. McElroy, M.B. Zeller, "Validation of the Chalk River Method of Analyzing Substitution Experiments by Comparison with Full-Core Measurements Volume II: Results", FFC-RRP-97, 1999 April.

13. R.S. Davis, A. Celli, J. Griffiths, R.T. Jones, D.C. McElroy, M.B. Zeller, "Validation of the Chalk River Method of Analyzing Substitution Experiments by Comparison with Full-Core Measurements Volume III: Conclusions", FFC-RRP-97/COG-98-38/ Volume III, 1999 April.

14. A. Celli, R.S. Davis, S.R. Douglas, R.T. Jones, D.C. McElroy, M.B. Zeller, "Validation of the Substitution Method for Determining Critical Bucklings, with Application to Natural Uranium and Simulated Burnup CANDU Fuel", COG-99-38, FFC-RRP-156, 2000 July.

15. D.V. Altiparmakov, "An Addition to WIMS-AECL ENDF/B-VI-based Library to Include Dysprosium Burnup Chain", FFC-RRP-365, AECL, 2001 June.

16. R.S. Davis, "Conifers: A Neutronics Program for Reactors with Channels, Revision 1, AECL-5305, 1998 July. (The executable and code sourceof Conifers is also requested).

17. R.S. Davis, "Why and How to Improve Accuracy in Conifers, RFSP, and Other Reactor Codes", Memo RRP-03-39, 2003 April 9.

Table 2. Required nuclear data for ACR-700 analysis

O16; KR83; ZR93; MO95; M097; MO100; TC99; RU101; RU102; RU103
RH103; RH105; PD105; PD107; PD108; AG109; CD113; IN115; I129; I135
XE131; XE133; XE135; CS133; CS134; CS135; LA139; CE141; CE142; CE144;
PR141; PR143; ND143; ND144; ND145; ND146; ND147; ND148; PM147;
PM148; PM148M; PM149; PM151; SM147; SM149; SM150; SM151; SM152;
EU153; EU154; EU155; EU156; GD157; DY160; DY161; DY162; DY163;
DY164; HO165; ER166; ER167; U233; U234; U235; U236; U238; NP237;
NP238; NP239; PU236; PU238; PU239; PU240; PU241; PU242; AM241;
AM242M; AM243; PFP; PFP2

Table 3. Available covariance data in ENDF/B

Nuclides	ENDF/B-V	ENDF/B-VI
^{1}H	Y	
^{6}Li	Y	
^{7}Li	Y	Y
^{10}B	Y	
C	Y	Y
^{14}N	Y	
^{16}O	Y	
^{19}F	Y	Y
^{23}Na	Y	Y
^{27}Al	Y	Y
^{28}Si, ^{29}Si, ^{30}Si, Si (natural)	Y	Y
^{45}Sc		Y
^{46}Ti, ^{47}Ti, ^{48}Ti		Y
V		Y
^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr		Y
Cr (natural)	Y	
^{55}Mn	Y	Y
^{54}Fe, ^{56}Fe, ^{57}Fe, ^{58}Fe		Y
Fe (natural)	Y	
^{59}Co	Y	Y
^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, ^{64}Ni		Y
Ni (natural)	Y	
^{63}Cu, ^{65}Cu		Y
^{89}Y		Y
^{93}Nb		Y
In, ^{115}In		Y
^{185}Re, ^{187}Re		Y
^{197}Au	Y	Y
^{206}Pb, ^{207}Pb, ^{208}Pb		Y
Pb (natural)	Y	
^{209}Bi		Y
^{232}Th	Y	Y
^{235}U, ^{238}U	Y	Y
^{237}Np	Y	
^{239}Pu	Y	
^{240}Pu, ^{241}Pu, ^{242}Pu	Y	Y
^{241}Am	Y	Y

Table 4-a. Nuclides in SCALE ENDF/B-V covariance library

Identifier	Isotope	Identifier	Isotope
13027	Al-27	11023	Na-23
95241	Am-241	28000	Ni
79197	Au-197	92237	Np-237
5010	B-10	8016	O-16
6012	C-12	82000	Pb
27059	Co-59	94239	Pu-239
24000	Cr	94240	Pu-240
9019	F-19	94241	Pu-241
26000	Fe	94242	Pu-242
1001	H-1	14000	Si
49115	In-115	90232	Th-232
3006	Li-6	92235	U-235
3007	Li-7	92238	U-238
25055	Mn-55	98252	Cf-252
7014	N-14		

Table 4-b. Nuclides in SCALE expanded covariance library

Identifier	Isotope	Identifier	Isotope
47109	Ag-109	60143	Nd-143
95243	Am-243	60145	Nd-145
55133	Cs-133	94238	Pu-238
29000	Cu	45103	Rh-103
63153	Eu-153	44101	Ru-101
63154	Eu-154	62147	Sm-147
63155	Eu-155	62149	Sm-149
64154	Gd-154	62150	Sm-150
64155	Gd-155	62151	Sm-151
64156	Gd-156	62152	Sm-152
64157	Gd-157	43099	Tc-99
72000	Hf	92233	U-233
19000	K	92234	U-234
12000	Mg	92236	U-236
42095	Mo-95	40000	Zr