

AECL

REFERENCE 5

**RESULTS OF A SURVEY ON ACCIDENT AND SAFETY ANALYSIS CODES,  
BENCHMARKS, VERIFICATION AND VALIDATION METHODS**

by

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## 1. INTRODUCTION

During the "Workshop on R&D Needs" at the 3<sup>rd</sup> Meeting of the International Group on Research Reactors (IGORR-III), the participants agreed that it would be useful to compile a survey of the computer codes and nuclear data libraries used in accident and safety analyses for research reactors and the methods various organizations use to verify and validate their codes and libraries. The following organizations submitted information for this survey:

Atomic Energy of Canada Limited (AECL, Canada),  
China Institute of Atomic Energy (CIAE, Peoples Republic of China),  
Japan Atomic Energy Research Institute (JAERI, Japan),  
Oak Ridge National Laboratories (ORNL, USA), and  
Siemens (Germany).

## 2. DEFINITION OF BENCHMARK, VERIFICATION AND VALIDATION

In their submissions the various organizations refer to "benchmark" methods and calculations, "validation" work, and "verification" for computer codes and libraries. The authors of this survey have attempted to compile a consistent survey by applying a consistent definition to those terms:

**Verification:** confirms that the intended equations, initial conditions, and boundary conditions are correctly programmed and perform as intended.

**Validation:** confirms, via comparison to available measurements, that the equations as programmed capture reality with a sufficient degree of fidelity.

**Benchmark:** a standard problem set with known or mutually agreed upon results used to verify a computer code, or a standard set of measured data used to validate a given application of the computer code.

## 3. NATIONAL STANDARDS

Several organizations submitted information about their national standards for software quality assurance and examples of how those standards are implemented for specific

research reactor projects:

**Canada:** AECL is currently implementing a software quality assurance (SQA) program based on the requirements set out in the Canadian Standards Association (CSA) N286.7-94 standard [1]. This standard covers the development of new software, the use of existing software, and the modification of existing software, where such software is used in support of safety related nuclear systems. The term software includes the encoding of correlations and mathematical methods and the data input to the models. Each specific nuclear project is required to develop and implement a project-specific quality assurance plan that encompasses all activities within the project. In addition to providing procedures for a SQA program, all design calculations or calculations to provide input to design are executed in accordance with design procedures based on CSA N286.2-86 [2]. As a specific example, the Research-Reactor Technology Branch (RTB) in AECL has implemented a SQA program [3] for the computer codes, data libraries and input models used to analyze research reactor concepts such as the proposed Irradiation Research Facility [4].

**China:** The submission [5] from the CIAE stated that China issued the Nuclear Industry Standards, EJ/T617-91, "A Guide to Verification and Validation for Computer Software Codes in Nuclear Industry Science and Engineering," in 1991. This standard is equivalent to the American National Standards, ANSI/ANS 10.4-1987. Implementation of a SQA program for verification and validation of computer codes is at an early stage.

**Germany:** The submission [6] from Siemens did not mention any specific standard for SQA. However, two computer software systems for performing nuclear design calculations, MARS and RSYST, are described. The MARS system was developed at Siemens/INTERATOM, whereas the RSYST system was developed at IKE-Stuttgart and at the Computer Centre at the University of Stuttgart. The MARS system and two versions, RSYST-I and RSYST-III, of the RSYST system have been used for the nuclear design of the FRM-II. Two different code systems were used to provide a broad verification of the nuclear design of the FRM-II.

**Japan:** The Japanese did not indicate any specific standard for SQA [7] is in use. However, JAERI uses a standard neutronic code system, SRAC (Standard Thermal Reactor Nuclear design code system) [8], for any type of thermal reactors.

**USA:** At ORNL, the ANS (Advanced Neutron Source) Project has implemented a SQA program [9] based principally on the requirements of Supplements 3S-1 and 11S-2 of the NQA-1 standard [10] and of Part 2.7 of the NQA-2 standard [11]. In addition, the ANS Project is committed to being judged licensable under the standards applied by the US Nuclear Regulatory Commission (NRC).

#### **4. METHODS AND CODES USED IN ACCIDENT AND SAFETY ANALYSIS**

##### **4.1 COMPUTER CODES AND METHODS FOR STATIC NEUTRON PHYSICS CALCULATIONS**

Each organization participating in the survey provided information on their computer codes for performing:

- **Cell calculations:** These codes are used to perform spectral calculations in the cells and to produce condensed few-group constants, macroscopic absorption and fission cross sections, and macroscopic reaction rates for use in the core calculations. Two calculational methods are generally used, discrete ordinates transport theory and the collision probability form of the transport equation.
- **Core calculations:** Three calculational methods are generally used, diffusion theory, discrete ordinates transport theory and Monte Carlo theory, to solve the Boltzmann transport equation. The CIAE also use the nodal method to calculate criticality, flux and power distributions, and reactivity coefficients.

The computer codes and methods are listed in Table 1. The RSYST code system [6] contains a sequence of modules for microscopic library compilation, macroscopic constant generation, performing spectral cell calculations. This has been represented in Table 1 by referring to RSYST rather than including the names of the specific modules. The same has been done for the AMPX/SCALE [12,13] code system. The WIMS-AECL [14] and WIMS-D4 codes use both discrete ordinates transport theory and the collision probability form of the transport equation.

As shown in Table 2, the key core performance parameters are generally calculated using different methods to provide independent verification of the results. The only exception is in the case of fuel depletion calculations where only diffusion theory is generally used to estimate the core burnup.

Most of the computer codes listed in Tables 1 and 2 have a long history of applications in many projects. Nevertheless, the SQA programs for many recent research reactor projects (e.g., ANS and IRF) require that the computer codes used for design calculations and safety analyses be verified and validated for the specific applications. Verification of the computer codes are addressed as follows:

- AECL relies on benchmark problems, inter-code comparisons and verification reports from code maintainers; the software includes in-house development (e.g., WIMS-AECL) and international sources (e.g., 3DDT, MCNP and DANTSYS),

Table 1: Summary of Computer Codes and Methods

METHOD	AECL	CIAE	JAERI	ORNL	Siemens
Cell calculation - collision probability - transport	WIMS-AECL	WIMS-D4  PASC-1	PIJ  ANISN TWOTRAN [22]	AMPX/ SCALE	RSYST, MONSTRA
Core calculation - diffusion	3DDT [15]	CITATION [19] EXTERMINATOR-2 [20]	CITATION	VENTURE [23]	DIF1D, DIF2D DIXY
- Monte Carlo	MCNP [16] KENO [13]	MCNP	MCNP	MCNP KENO	MORSE-K MOCA
- transport	DANTSYS [17,18]	ANISN [21] DOT3.5	ANISN TWOTRAN	DORT [24]	IANISN, SN1D DOT
- nodal method		PSUI- LEOPARD/ NGMARC			

Table 2: Summary of the Codes Used to Calculate Key Physics Parameters

Parameter	AECL	CIAE	JAERI	ORNL	Siemens
k-effective	3DDT MCNP	MCNP ANISN DOT3.5 PSUI- LEOPARD/N GMARC	CITATION TUD TWOTRAN MCNP	MCNP KENO DORT	MORSE-K MOCA DOT
reactivity worth	3DDT MCNP DANTSYS	MCNP	ANISN TWOTRAN MCNP	MCNP	MORSE-K MOCA DOT
reactivity coefficients	3DDT	CITATION ANISN DOT3.5	CITATION TUD ANISN TWOTRAN	VENTURE DORT	DIF2D
flux and power distributions	3DDT MCNP	CITATION MCNP ANISN DOT3.5	CITATION TUD ANISN TWOTRAN	VENTURE MCNP DORT	DIF2D MORSE-K DOT
fuel depletion	3DDT/ FULMGR	CITATION/ 2DFGD EXTERMINATOR-2	CITATION TUD	VENTURE/ BURNER	RSYST MARS

- CIAE relies on software obtained from international sources (e.g., RSIC, NESC, NEA),
- JAERI has verified SRAC system using international benchmark problems,
- ORNL relies on verification reports from code developers (e.g., ORNL, LANL) for the ANS Project, and
- Siemens relies on inter-code comparisons between the RSYST and MARS systems for FRM-II.

Validation of the computer codes are addressed as follows:

- **AECL:** Code validation relies on comparisons against benchmark problems, inter-code comparisons and comparisons against critical experiments. For the current work on research reactor projects (e.g., IRF) in AECL, RTB has been undertaking a validation program for the set of computer codes routinely used to perform design calculations and safety analyses. A validation report [25] has been produced to compile information pertaining to comparisons of WIMS-AECL predictions against:
  - CANDU-type fuel assemblies in a variety of coolant types (e.g., D<sub>2</sub>O, H<sub>2</sub>O, D<sub>2</sub>O/H<sub>2</sub>O mixtures, void and organic) using the ZED-2 critical facility,
  - burnup and isotope depletion data from CANDU fuel bundles discharged from the Bruce and Pickering power reactors, and
  - the R1/100H lattice experiments for H<sub>2</sub>O coolant temperature and density effects.

The WIMS-AECL/3DDT code set has also been validated [25] against the SPERT-1B reactor experiments for k-effective, reactivity coefficients and kinetics parameters, and the TRX experiments for k-effective. A similar report has compiled validation data for MCNP [26]. For example, MCNP has been validated against commissioning data from the SLOWPOKE Demonstration Reactor for k-effective and gamma dose rates [27]. The need for further validation work will depend on the specific requirements of a research reactor project.

- CIAE relies on IAEA benchmarks.
- JAERI relies on IAEA benchmarks (e.g., IAEA 10 MW Benchmark Reactor [28]) and critical experiments and JRR-3 commissioning data. The information from JAERI indicated that the SRAC system had been validated against many critical experiments (e.g., Tank-type Critical Assembly for light-water reactors,

Deuterium Critical Assembly for the Advanced Thermal Reactor for H<sub>2</sub>O-cooled and D<sub>2</sub>O-moderated reactors, Semi-Homogeneous Experimental facility for 20 wt% enriched uranium in a graphite moderator, JMTRC critical facility for JMTR, TRX experiments and a series of FBR cores). Comparisons have also been made against international benchmarks developed for the RERTR (Reduced Enrichment for Research and Test Reactor) program (e.g., LEU initial core for the Ford Nuclear Reactor), and temperature and void coefficient measurements in KUCA.

- ORNL has validated their computer codes for the ANS Project against:
  - Los Alamos critical mass data for enriched uranium in bare H<sub>2</sub>O- and D<sub>2</sub>O-reflected critical experiments, ORNL H<sub>2</sub>O-solution critical experiments, and D<sub>2</sub>O-moderated, natural uranium ZEEP critically-buckled lattices,
  - FOEHN critical experiments [29] to validate predictions from MCNP, VENTURE/BURNER, DORT and KENO,
  - ANS critical experiments to supplement validation from the FOEHN experiments, and
  - HFIR and ILL operating data to validate the fuel depletion calculations.
- Siemens has commissioning data from RSG-GAS-30 (Indonesia) for validation.

#### 4.2 NUCLEAR DATA LIBRARIES

The survey identified the list of nuclear data libraries listed in Table 3 are being used for physics calculations. For the ANS Project, a dedicated multigroup nuclear library, ANSL-V, was prepared from the ENDF/B-V library, and validated [7]. Verification and validation of the nuclear data libraries are combined with the verification and validation of the codes.

#### 4.3 COMPUTER CODES AND METHODS FOR THERMALHYDRAULIC AND TRANSIENT ANALYSIS

The information from the participants in the survey identified the following thermalhydraulics codes in use for accident analyses:

**AECL:** CATHENA [30] is a two-fluid (6 equation) code used for the dynamic simulation of reactor transients involving thermalhydraulics and kinetics. It was originally developed for the fluid conditions in a CANDU reactor and subsequently modified for use with MAPLE-X10 coolant conditions. Heat transfer correlations for the MAPLE-X10 coolant conditions were obtained from heat transfer experiments using electrically-heated fuel-element simulators in a flow test rig. Work is in progress to extend those heat transfer correlations to cover the expected coolant conditions for the IRF.



Table 3: Summary of Nuclear Data Libraries and Computer Codes

LIBRARY	AECL	CIAE	JAERI	ORNL	Siemens
CSRL-IV		PASC-1			
ENDF/B-IV	KENO	MCNP	ANISN, PIJ TWOTRAN		MONSTRA CGM
ENDF/B-V	WIMS- AECL MCNP		MCNP	AMPX/SCALEDO RT VENTURE/ BURNER MCNP, KENO	CGM
ENDF/B-VI	WIMS- AECL				
GAM/ THERMOS		PASC-1			
JEF1					CGM
JENDL-2			PIJ, TWOTRAN		
VITAMIN-C		PASC-1			
WINFRITH	WIMS- AECL	WIMS-D4			

**CIAE:** The information from the CIAE indicated that they are using a code called THAS-PC4, modified from COBRA-IV, to perform steady-state thermalhydraulic analyses for the CARR Project. Thermalhydraulic accident analyses for the CARR Project will be performed using RETRAN-02.

**JAERI:** JAERI used HEATING-5 [31], EUREKA-2 [32] and THYDE-P [33] for thermalhydraulic analyses for the upgraded JRR-3 reactor. HEATING-5 is designed to solve steady-state and transient heat conduction problems in one-, two-, or three-dimensional Cartesian or cylindrical coordinates. EUREKA-2 provides a coupled thermal, hydraulic and point kinetics capability for evaluating a postulated reactivity initiated transient. THYDE-P is designed to analyze anticipated operational transients and accident conditions in light-water power reactors. JAERI modified the heat transfer correlations and the DNB (departure from nucleate boiling) correlations [34] for the thermalhydraulic design and safety analysis of the upgraded JRR-3.

**ORNL:** For the ANS Project, RELAP5 [35] is used for the thermalhydraulic design of the cooling systems. RELAP5 has been verified by INEL (Idaho National Engineering Laboratory), and the ANS Project planned to validate it against HFIR, the Thermal-Hydraulic Test Loop [36] and a planned integral test facility.

CONQUEST is planned to be used for reactivity initiated transients. It has been verified against IAEA benchmarks and it was planned to validate CONQUEST against measurements from the planned ANS critical facility.

## 5. SUMMARY

This report is a compilation of the information submitted by AECL, CIAE, JAERI, ORNL and Siemens in response to a need identified at the "Workshop on R&D Needs" at the IGCRR-III meeting. The survey compiled information on the national standards applied to the SQA programs undertaken by the participants. Information was assembled for the computer codes and nuclear data libraries used in accident and safety analyses for research reactors and the methods used to verify and validate the codes and libraries. Although the survey was not comprehensive, it provides a basis for exchanging information of common interest to the research reactor community.

## REFERENCES

1. "Quality Assurance for Analytical, Scientific and Design Computer Programs for Nuclear Power Plants," Canadian Standards Association, CSA-N286.7-94, 1994 June (draft).
2. "Design Quality Assurance for Nuclear Power Plants," Canadian Standards Association, CSA-N286.2-86, 1986.
3. G.B. Wilkin, "Research-Reactor Technology Branch Quality Assurance: Computer Software Control and Application Procedures," AECL Report, RC-2000-063(Rev. 1), 1995 May.
4. R.F. Lidstone, A.G. Lee, W.E. Bishop, E.F. Talbot, AND H. McIlwain, "Development of the New Canadian Irradiation-Research Facility," Proceedings of the 4<sup>th</sup> Meeting of the International Group on Research Reactors, Gatlinburg, Tennessee, 1995 May 24-25.
5. Yuan Luzheng, "China Advanced Research Reactor (CARR) Code Verification and Validation for Methods used in Accident and Safety Analysis," CIAE Report, 1995.
6. Feltes, "Comprehensive Description of the Computer Code and Calculation Processes in the Core Design," ORNL Report, ORNL/OLS-94/12, translated from the German Siemens Arbeits-Bericht [Project Report], Report No. KWU BT 14/94/315, 1994 June.

7. "Benchmark Methods, Safety Analysis Methods, Code for Licensing and Safety Authorities for Research Reactors in JAERI."
8. K. Tsuchihashi, Y. Ishiguro, K. Kaneko and M. Ido, "Revised SRAC Code System," JAERI-1302, 1986.
9. "Advanced Neutron Source (ANS) Code Verification and Validation for Methods used in Accident and Safety Analysis."
10. "Supplementary Requirements for Design Control," Supplement 3S-1 and "Supplementary Requirements for Computer Program Testing," Supplement 11S-2 *Quality Assurance Requirements for Nuclear Facility Applications*, ASME NQA-1-1989 Edition (Revision of ASME NQA-1-1986 Edition), American Society of Mechanical Engineers, 1989 September 15.
11. "Quality Assurance Requirements of Computer Software for Nuclear Facility Applications," ASME NQA-2a-1990, Addenda to *Quality Assurance Requirements for Nuclear Facility Applications*, ASME NQA-2-1989 Edition (Revision of ASME NQA-2-1986 Edition), American Society of Mechanical Engineers, 1989 September 30.
12. N.M. Greene et al, "AMPX-77: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Cross-Section Libraries from ENDF/B-IV and/or ENDF/B-V," ORNL Report, ORNL/CSD/TM-283, 1992 October.
13. "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," ORNL Report, NUREG/CR-0200 Rev.4 (ORNL/NUREG/CSD-2/R4), 1993 November.
14. J. Griffiths, "WIMS-AECL User's Manual," AECL/COG Report, RC-1176/COG-94-52, 1994 March.
15. J.C. Vigil, "3DDT, a Three-dimensional Multigroup Diffusion-burnup Program," Los Alamos Scientific Laboratories report, LA-4396, 1970 February.
16. J.F. Briesmeister, ed., "MCNP - A General Monte Carlo N-Particle Transport Code, Version 4A," Los Alamos National Laboratories Report, LA-12625, 1993 November.
17. F.W. Brinkley, "TWO-DANT-SYS: One- and Two-Dimensional, Multigroup Discrete-Ordinates Transport Code System," RSIC computer code CCC-547/TWO-DANT-SYS (1990), LANL Reports: LA-9184-M, ANNUITANT (1989); LA-10258-M, TWOHEX (1989); LA-10049-M, TWO-DANT (1990).

18. R.E. Alcouffe, F.W. Brinkley and D.R. Marr, "User's Guide for THREEDANT: A Code Package for Three-Dimensional, Diffusion-Accelerated, Neutral-Particle, Transport," LANL Report, LA-10049-M (1990).
19. T.B. Fowler, D.R. Vondy and G.W. Cunningham, "Nuclear Reactor Core Analysis Code: CITATION," ORNL Report, ORNL-TM-2496 Rev. 2, 1971 July.
20. T.B. Fowler, M.L. Tobias and D.R. Vondy, "Exterminator-II, A FORTRAN-IV Code for Solving Multigroup Diffusion Equations in Two Dimensions," ORNL Report, ORNL-4078, 1967.
21. W.W. Engle, Jr., "A User's Manual for ANISN: A One Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," K-1693, 1976.
22. R.E. Alcouffe, F.W. Brinkley, D.R. Marr and R.D. O'Dell, "User's Guide for TWOTRAN: Two-Dimensional Diffusion Accelerated Discrete-Ordinates Transport Code," LANL Report, LA-10049-M, 1984 February.
23. D.R. Vondy, "VENTURE: A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-Difference Diffusion Theory Approximation to Neutron Transport," ORNL Report, ORNL-5602, 1975.
24. W.A. Rhodes and R.L. Childs, "The DORT Two-Dimensional Discrete Ordinates Transport Code," Nuclear Science and Engineering, **99**, 88 (1988).
25. P.A. Carlson, "Validation of WIMS-AECL and WIMS-AECL/3DDT for Research Reactor Applications," AECL Proprietary Report, RTB-TN-018, 1994 December.
26. H. McIlwain, "Validation of MCNP for Research Reactor Applications," AECL Proprietary Report, RTB-TN-040, 1994 December.
27. H. McIlwain, "Validation of MCNP Using SDR Critical Data and Gamma Dose Rate Measurements," AECL Report, RTB-TN-046, 1995 April.
28. "Research Reactor Conversion from the Use of Highly Enriched Uranium to the Use of Low Enriched Uranium Guidebook," IAEA-TECDOC-233, 1980.
29. A.M. Ougouag et al, "MCNP Analysis of the FOEHN Critical Experiment." ORNL Report, ORNL/TM-12466, 1993 October.
30. D.J. Richards, B.N. Hanna, N. Hobson, and K.H. Ardron, "ATHENA: A Two-Fluid Code for CANDU LOCA Analysis," Proceedings of the Third International Topical Meeting on Reactor Thermalhydraulics, Newport, Rhode Island, 1985 October 15-18. *(the code has been renamed CATHENA)*

31. W.D. Turner, D.C. Elrod and I.I. Siman-Tov, "HEATING-5-An IBM 360 Heat Conduction Program," ORNL Report, ORNL/CSD/TM-15.
32. N. Onishi, T. Harami, H. Hirose and M. Uemura, "A Computer Code for the Reactivity Accident Analysis in a Water Cooled Reactor," JAERI Report, JAERI-M 84-074, 1984.
33. Y. Asahi, "Description of THYDE-P (Preliminary Report of Methods and Models)," JAERI Report, JAERI-M 7751, 1978.
34. Y. Sudo, H. Ikawa and M. Kaminaga, "Development of Heat Transfer Package for Core Thermal-hydraulic Design and Analysis of Upgraded JRR-3," Proceedings of the International Meeting of Reduced Enrichment for Research and Test Reactors, Petten, the Netherlands, 1985 October 14-16.
35. K.E. Carlson et al, "RELAP5/MOD3 Code Manual, Volume 1: Code Structure, System, Models, and Solution Methods," INEL Report, NUREG/CR-5535 (EGG-2596), 1990 June.
36. D.K. Felde et al, "Advanced Neutron Source Thermal-Hydraulic Test Loop Facility Description," ORNL Report, ORNL/TM-12397, 1994 February.