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SHIELD VERIFICATION AND VALIDATION ACTION MATRIX SUMMARY (U)

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TITLE: SHIELD VERIFICATION AND VALIDATION ACTION MATRIX SUMMARY (U).

TASK: CERTIFICATION PLAN FOR SHIELD (91-013-1)

APPROVALS

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1.0 SUMMARY

WSRC-RP-90-26, *Certification Plan for Reactor Analysis Computer Codes (U)* (Ref. 1), describes a series of action items to be completed for certification of reactor analysis computer codes used in Technical Specifications development and for other safety and production support calculations. Validation and verification are integral part of the certification process (Ref. 2). This document identifies the work performed and documentation generated to satisfy these action items for the SHIELD, SHLDED, GEDIT, GENPRT, FIPROD, FPCALC, and PROCES modules of the SHIELD system, it is not certification of the complete SHIELD system. Complete certification will follow at a later date. Each action item is discussed with the justification for its completion. Specific details of the work performed are not included in this document but can be found in the references. The validation and verification effort for the SHIELD, SHLDED, GEDIT, GENPRT, FIPROD, FPCALC, and PROCES modules of the SHIELD system computer code is completed.

2.0 INTRODUCTION

WSRC-RP-89-1249, *Verification and Validation Plan for Reactor Analysis Computer Codes* (Ref. 2), describes a series of action items to be completed for verification and validation of reactor analysis computer codes used in Technical Specifications development and for other safety and production support calculations. These requirements have been organized into an action matrix. Each action item describes the different type of information and documentation that must be assembled for each code to be certified. The action matrix serves as a useful tracking tool for monitoring completion of the certification process for individual codes.

Figure 1 shows the present status of the action matrix for the the SHIELD, SHLDED, GEDIT, GENPRT, FIPROD, FPCALC, and PROCES modules of the SHIELD system computer code. As can be seen in the figure, all the requirements for verification and validation of the code have been completed with the exception of the review process. The rest of this document gives the justification for checking each box in turn and identifies all relevant reference documentation.

The action matrix (Figure 1) divides the activities into five groups: Basics, Theory, Experiments, Benchmarks, and Conclusions. The remainder of this report utilizes the same structure and format.

3.0 ACTION MATRIX

3.1 BASIC REQUIREMENTS

3.1.1 User's Manual in Place

User documentation for the SHIELD computer code is contained in the The SHIELD System User's Manual (Ref. 3). This document provides all the necessary information for knowledgeable individuals to utilize the SHIELD code providing they are familiar with the WSRC computer facilities and the JOSHUA (Ref. 4) system. The user's manual explains how to set up and interpret results from all of the important calculations performed using the SHIELD code.

Chapters I and II of the user's manual present an introduction and overview of the SHIELD system and of the associated supporting nuclear data libraries. These chapters also describe the general class of problems that can be solved with the SHIELD system. Chapter III describes the conventions used to execute a problem using the SHIELD system. Detailed input instructions for the individual calculation types are described in chapter IV. Chapter V lists references.

Following the five chapters are a series of appendices: Appendix A provides information on the nuclear data base; Appendix B describes test problems; Appendix C documents validation studies; Appendix D documents the SHIELD system input record formats; Appendix E describes support data sets and record formats; and, Appendix G provides documentation on the peer review of the SHIELD system.

In addition to the user's manual, a SHIELD User's Notice (Ref. 5) has been issued which provides information about the location of the J80 version of SHIELD, instructions for executing SHIELD, information about user levels, and training requirements.

3.1.2 Configuration Control Plan

The Configuration control plan for the reactor analysis computer codes, including the SHIELD code, is given in the *Certification Plan for Reactor Analysis Computer Codes* (Ref. 1). Configuration control of the SHIELD code is implemented by following Procedure No. TP-90-018: *Responsibilities of Technical Proprietors for Configuration Management Using SCMS* (Ref. 6). A configuration controlled version of SHIELD on the IBM 3090 under the J80 version of JOSHUA has been installed. The source code for the SHIELD system modules currently being certified is stored under the Scientific Code Management System, which protects it from unauthorized changes, and ensures strict quality assurance standards are adhered to. The source listing for the SHIELD, SHLDED, GEDIT, GENPRT, FIPROD, FPCALC, and PROCES modules of the SHIELD system are located on the VAX cluster, in the SCMS libraries SRLUSER3:[SCMS.SOURCE.SHIELD]. The executable J80 version of SHIELD has also been stored under the Scientific Code Management System. The executable SHIELD, SHLDED, GEDIT, GENPRT, FIPROD, FPCALC, and PROCES modules are located on the IBM 3090 in the data set USCS.SCMS.LOAD.

Instructions for executing SHIELD on the IBM under J80 can be found in Ref. 5. A set of test problems has been developed which span the range of applications of the SHIELD modules being certified. The input and output from these problems are detailed in Ref. 7. The test problems can be found on the IBM in the data set USCS.SCMS.TEST.

3.1.3 Code Portability

SHIELD has been converted to standard FORTRAN 77, a machine independent language. However, SHIELD is intimately tied to the JOSHUA system, which is machine dependent. Therefore, the portability of SHIELD is dependent upon the portability of the JOSHUA system. SHIELD, and the JOSHUA system, were originally written on the IBM mainframes at the SRS; currently they run on the IBM 3090. Limited portability of JOSHUA has been demonstrated and additional portability can be implemented if the need arises.

3.2 VERIFICATION OF THEORY

3.2.1 Appropriate Theory

The theory of the FIPROD, FPCALC and PROCES modules are described here.

The decay and/or buildup of radioactive nuclides under conditions of spontaneous decay is solved by modules FIPROD and FPCALC. The FIPROD module calls the FPCALC module to perform the actual production-depletion calculation using either the linearized chain or matrix exponential mathematical algorithms. The time dependent isotopic composition is solved for using a first order differential equation for burnup. The FPCALC module being certified here assumes space independent fluxes and cross sections, or that any space dependence of fluxes and cross sections has been averaged into the input information. FIPROD is also capable of performing a cooling calculation which computes the isotopic inventory of radionuclides under zero-flux conditions.

Two mathematical algorithms are available in the FIPROD module for the burnup or cooling calculations. The LINCHAIN option approximates the coupling matrix between isotopes to a vector representation and solves the vector problem by an explicit solution. This mathematical algorithm is similar to that used in the CINDER code (Ref. 9). The MATEXP option uses the matrix exponential approximation to the full matrix solution. This mathematical algorithm is the same used in the ORIGEN code (Ref. 10).

The PROCES module of the SHIELD system simulates the mechanical and chemical fuel cycle processes. The quantity conserved in the normal fuel cycle calculation is the total mass of each isotope that enters and leaves a process vessel. More detailed solution method descriptions of FIPROD, FPCALC, and PROCES can be found in Ref. 3, The SHIELD System User's Manual.

The theory described above are all industry accepted approaches (Ref. 11 &12). The theory employed by the SHIELD code is appropriate for the types of problems it is intended to solve.

3.2.2 Theory Documented

The SHIELD code theory documented in Ref. 3 is described in detail in standard nuclear analysis methodology texts such as Refs. 11 & 12. Since no new theoretical development is introduced, the basic theory as documented in the open literature provides conceptual verification of the code theory as required.

3.2.3 Coding Consistency

The SHIELD code was developed long before the current validation and verification requirements were in place and as a result the verification performed at the time was not documented sufficiently to meet current requirements. Retroactively verifying line by line the coding of such a large software system as SHIELD would be a monumental task and it has not been deemed necessary. The extensive operations history of SHIELD, in conjunction with the code validation discussed below, is sufficient to establish that the code is functioning as intended and therefore this item is satisfied.

3.2.4 Theory Verified Conceptually

The SHIELD code theory is summarized in Ref. 3. Since no new theoretical development is introduced, the basic theory as documented in the open literature and the description of the code function provide conceptual verification of the code theory as required.

3.2.5 Theory Verified by Experiment

The SHIELD code was developed long before the current validation and verification requirements were in place and as a result the verification performed at the time was not documented sufficiently to meet current requirements. The extensive operations history of SHIELD, however, in conjunction with the code validation discussed below is sufficient to establish that the code is functioning as intended. The validation process is described in *SHIELD Verification and Validation Report* (Ref. 13).

3.2.6 Theory Documentation Adequate

The techniques employed by the applicable SHIELD modules are well documented in the open literature. The documentation is adequate to demonstrate the adequacy of the theory.

3.3 VALIDATION WITH EXPERIMENTS

3.3.1 Tests in Experimental Facilities

Tests have been performed in experimental facilities at Oak Ridge National Laboratory (ORNL) and Los Alamos National Laboratory (LANL) and the results have been used to validate SHIELD (Refs. 14-16).

3.3.2 Tests in Operating Facilities

No tests in operating facilities were used for the validation of SHIELD. This item is not required for validation because other means of validation have been demonstrated.

3.3.3 Data from Operating Facilities

Measurements were made in the SRS separations area for fission product activities in discharged Mark 22, 16B and 53B assemblies and decay heat in Mark 22, 16B, 31A and 31B assemblies (Refs. 17-20).

3.3.4 Test Data Documented

A body of data has been identified and documented (Refs. 3 & 14-20). Conditions under which the data were collected can be determined with reasonable assurance in the references. Documentation of these test are in the open literature.

3.3.5 Appropriate Data Quality

All relevant experimental and operating data were taken prior to present QA standards being adopted. Standard data acquisition methods and techniques were used in experimental facilities at LANL, ORNL and SRS.

3.3.6 Validation Performed

The SHIELD code has been validated against both experimental and operating data. The code features and models that have been validated are described in *SHIELD Verification and Validation Report* (Ref. 13), and the actual validations are summarized in earlier validation documents (Ref. 3 & 21). These documents received in-depth technical reviews.

3.3.7 Validation Documentation Adequate.

This item was satisfied by technical review of the *SHIELD Verification and Validation Report* (Ref. 13).

3.4 VALIDATION BY BENCHMARKING

3.4.1 Benchmark Requirements Identified

Benchmark requirements are listed in Ref. 3.

3.4.2 Similar Code Comparison

The FIPROD and FPCALC calculations were compared to CINDER (Ref. 9) and ORIGEN (Ref. 10) results as documented in the *SHIELD Verification and Validation Report* (Ref. 13).

3.4.3 Exact Solution Comparison

Sample problems for the PROCES and EDIT modules were made trivial so that hand calculations were possible for verification. Comparisons of PROCES results to hand calculations show exact agreement (Ref. 22).

3.4.4 Industry Benchmark Comparisons

No industry benchmark cases have been used in the validation of SHIELD. This item is not required for validation because other means of validation have been demonstrated.

3.4.5 Comparisons Documented

The results of the benchmarking are documented in the references given in *SHIELD Validation and Verification Report* (Ref. 13). Two documents in particular (Refs. 3 and 21 of this document) summarize most of this information and satisfy the documentation requirements.

3.4.6 Benchmark Documentation Adequate

The benchmark documentation contained in SHIELD *Validation and Verification Report* (Ref. 13) is adequate for validation of the SHIELD code.

3.4.7 Standard Set of Test Problems

A standard set of test problems has been developed and documented (Ref. 7). Complete input and output for these problems is provided in the documentation, and the test problems have been placed in protected data sets.

4.0 CONCLUSIONS

Verification and validation/benchmarking of the SHIELD code as outlined in Ref. 1 is now completed.

		RESULTS	INITIALS	DATE
Basics	**User Manuals in Place**	yes	CB	2/7/92
	Configuration Control Plan	yes	CB	2/12/92
	Code Portability	yes	CB	2/7/92
Theory	**Appropriate Theory**	yes	CB	2/7/92
	Theory Documented	yes	CB	2/7/92
	Coding Consistency	yes	CB	2/7/92
	Theory Verified Conceptually	yes	CB	2/7/92
	Theory Verified by Experiments	N/A	CB	2/7/92
	Theory Documentation Adequate	yes	CB	2/7/92
Experiments	**Tests in Experimental Facilities**	yes	CB	2/7/92
	Tests in Operating Facilities	N/A	CB	2/7/92
	Data from Operating Facilities	yes	CB	2/7/92
	Test Data Documented	yes	CB	2/7/92
	Appropriate Data Quality	yes	CB	2/7/92
	Validation Performed	yes	CB	2/7/92
	Validation Documentation Adequate	yes	CB	2/7/92
Benchmarks	**Benchmark Requirements Identified**	yes	CB	2/7/92
	Similar Code Comparison	yes	CB	2/7/92
	Exact Solution Comparison	yes	CB	2/7/92
	Industry Benchmark Comparison	N/A	CB	2/7/92
	Comparisons Documented	yes	CB	2/7/92
	Benchmark Documentation Adequate	yes	CB	2/7/92
Conclusions	**Verification review**	yes	CB	2/7/92
	Verification Completed	yes	CB	2/7/92
	Standard Set of Test Problems	yes	CB	2/7/92
	Validation/Benchmarking Review	yes	CB	2/7/92
	Validation/Benchmarking Completed	yes	CB	2/7/92

Verification and Validation Plan Action Matrix for SHIELD

Figure 1

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