

IMPROVEMENT AND QUALIFICATION OF WIMS UTILITIES

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Abstract

WIMS Utilities is a collection of FORTRAN programs and Perl files, used to post-process WIMS-AECL results and generate cross-section tables for use in RFSP-IST. Used routinely in safety analysis and core tracking, WIMS Utilities must comply with the CSA-N286.7-99 standard. Recent qualification activities, funded by Atomic Energy of Canada Limited (AECL) and the CANDU Owners Group (COG), include Software Quality Assurance (SQA) documentation for, and official release of, WIMS Utilities version 2.0, qualified for reactor physics analysis. This paper traces the development of WIMS Utilities version 2.0 by (a) identifying the qualification gaps identified in earlier versions; (b) discussing the development and qualification activities performed; and (c) demonstrating the qualification status achieved for WIMS Utilities 2.0.

1. Introduction

The Canadian nuclear industry has selected three reactor-physics computer codes for use in safety analysis, licensing, and routine operations for CANDU[®] nuclear reactors as documented in the IST (Industry Standard Toolset) agreement. These computer codes are WIMS-IST [1], RFSP-IST [2], and DRAGON-IST [3], used for 2-D lattice-cell transport calculations, 3-D core analysis, and 3-D supercell transport calculations, respectively. The three IST reactor-physics codes fit together to create a calculational system used for determining the neutron-flux distribution in CANDU reactors.

To accurately calculate the power distribution in the reactor core, RFSP-IST requires the few-energy-group lattice cross sections calculated with WIMS-IST in the form of fuel tables. However, WIMS-IST does not produce fuel tables in a format that can be used directly by RFSP-IST. The decision was made not to embed the specific data and formats required for each particular application of WIMS-IST in either the WIMS-IST code or a downstream diffusion code, such as RFSP-IST. Instead, the decision was made for WIMS-IST to write generic information to a binary TAPE16 file that could then be post-processed for the specific application required. The result was WIMS Utilities, developed to post-process the WIMS-IST TAPE16 file to generate WIMS-AECL tables – uniform parameter fuel/reflector tables, and Simple Cell Method (SCM) fuel/reflector tables – that could then be used in RFSP-IST.

WIMS Utilities has been developed and maintained at AECL and, for many years, was funded by the AECL R&D program. In 2005, the COG IST program (Work Package 51508) was initiated to fund and to participate in completing the qualification activities of WIMS Utilities.

This paper traces the development of WIMS Utilities version 2.0 by (a) identifying the qualification gaps and development needs identified in earlier versions (Section 2); (b) discussing the improvement and qualification activities carried out (Section 3); and (c) demonstrating the qualification status achieved for WIMS Utilities 2.0 in the conclusion (Section 4).

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2. WIMS Utilities Version 1.8 and Earlier

WIMS Utilities is a collection of FORTRAN programs and Perl script files. Each FORTRAN program, with actual numerical calculations involved, is task-specific, and was developed to post-process the WIMS-IST TAPE16 file for a specific application. The purpose of such a modular approach is to develop and qualify the post-processing utilities once, rather than re-invent and re-qualify the same post-processing operations many times for each particular application of WIMS-IST results.

WIMS Utilities version 1.8 and earlier were comprised of four major FORTRAN programs, two major Perl script files, and a number of minor programs.

The four FORTRAN utilities and their main functions were:

1. CONDENS Condensed the energy group structure of the data (cell-average data, multi-region data, and the isotopic microscopic cross sections) from fine to coarse energy groups.
2. MICROBURN Converted the isotopic reactions and/or reaction rates and neutron fluxes into isotopic microscopic cross sections over the whole cell or over selected regions of the cell.
3. REGAV Processed multi-region data into region-homogenized properties for a subset of regions in the original cell.
4. WRFSP Processed few-group, region-homogenized cross sections, saved in one or more existing TAPE16 files, to generate different types of fuel tables for use in RFSP-IST.

The two major Perl script files and their main functions were:

1. PROC16 Controlled the sequence of WIMS-IST calculations and post-processing. Calls the executables of WIMS-IST and the four major FORTRAN utilities (CONDENS, MICROBURN, REGAV, WRFSP) when required.
2. GEN_SIMP Prepared the input files for WIMS-IST and the four major FORTRAN utilities (CONDENS, MICROBURN, REGAV, WRFSP). Automates the preparation of the Simple Cell Method (SCM) tables.

WIMS Utilities version 1.8 also contained other minor utilities such as: LIST, CLIP, SMOOTH (all FORTRAN programs), and PMAT2LIB (a Perl script). Since these utilities do not involve scientific calculations, and since most of them comprise only a few lines of coding, they are not defined as scientific codes requiring qualification.

The CSA-N286.7-99 Standard [4] applies to the design, development, maintenance, modification and application of analytical, scientific, and design computer programs used in nuclear power plant operations to perform or support:

- a) the design and analysis of safety-related equipment, systems, structures and components as identified by the owner;
- b) deterministic and probabilistic safety analyses and reliability studies;

- c) reactor-physics and fuel-management calculations, and
- d) the transfer of data between computer programs or pre- or post-processing calculations associated with (a), (b) and (c) above.

Since numerical calculations are involved during post-processing in its FORTRAN programs and since WIMS Utilities is used routinely in safety analysis and core tracking, the program, regardless of version, satisfies all the items listed above and must therefore comply with CSA-N286.7-99.

Development of WIMS Utilities started prior to March 1999. Accordingly, WIMS Utilities qualifies as a legacy code, meaning that it is exempt from compliance with AECL QA procedures for some design and development activities. Even so, WIMS Utilities still has to satisfy the requirements for the application documents specified in the AECL Software Quality Assurance Manual (SQA Manual) and in N286.7-99.

WIMS Utilities version 1.8 was released before March 1999. A number of qualification gaps, user suggestions for improvement, and areas of non-compliance with new procedures were identified. These are discussed in the following subsections. Addressing these items – particularly the configuration management, platform, and documentation issues – led to the development of a new version: WIMS Utilities version 2.0.

2.1. WIMS Utilities Version 1.8 Qualification Gaps

2.1.1. Configuration Management

Configuration management deals with the obligation of code holders to ensure that the version of a computer program is applied appropriately and operates in a well-defined computing environment that is complete and consistent with its requirements. In other words, for a program to meet the qualification requirements for configuration management as outlined in AECL procedures, code holders would need to ensure that the documentation, executable, test suite, and source code for the program were all under configuration management.

In the case of WIMS Utilities version 1.8 on the HP-UNIX platform, AECL procedures had been revised so that the program was no longer compliant. For example, the utility version label was not given to each utility. This meant that work needed to be done to ensure compliance with new standards.

2.1.2 Platforms

A platform is a combination of computer architecture, operating system, programming languages and related runtime libraries or graphical user interfaces, which provide a distinct environment in which to write and execute a computer program.

For programs running on several different platforms, configuration management becomes more complex and more prone to error. While two independent sources of WIMS Utilities had been developed and maintained at AECL for two different platforms (HP-UNIX and PC Windows), users identified a need for WIMS Utilities on third platform, LINUX.

The decision was made to modify WIMS Utilities version 1.8 so that it would be platform independent. This would not only accommodate users running the program on different platforms but would also simplify configuration management of the program.

2.1.3 SQA Documentation

As a legacy code, WIMS Utilities is not subject to all the SQA documentation requirements of newer programs. Nonetheless, SQA documentation with respect to application documents was still mandated: Computer Program Abstract, Theory Manual, User's Manual, and Version Tracking Record.

These application documents were included in different AECL internal reports for CONDENS, GEN_SIMP, MICROBURN, PROC16, REGAV, and WRFSP. A validation report is not required, as it has already been covered in the validation document for the reactor-physics suite of codes (DRAGON/WIMS/RFSP).

Since WIMS Utilities had changed, however, documentation needed to be either updated or created to deal with these changes.

3. WIMS Utilities 2.0 Improvement and Qualification

Over the past several years, extensive development and qualification work regarding WIMS Utilities has been done. Section 3.1 describes the development effort that led to WIMS Utilities 2.0, while Section 3.2 recounts the qualification activities.

3.1. WIMS Utilities 2.0 Improvements

WIMS Utilities version 1.8 was originally designed to post-process the WIMS-AECL TAPE16 file generated from WIMS-AECL single lattice-cell calculations. To allow a more realistic calculation of lattice-cell properties for ACR[®] type fuel, the generic multicell calculation capability was developed in WIMS-AECL ver. 3.1 [5].

This led to changes, not only in the contents but also in the structure of WIMS-AECL TAPE16 records. In order to generate the conventional WIMS-AECL single-lattice-cell-based fuel tables and WIMS-AECL multicell fuel tables from WIMS-AECL version 3.1, WIMS Utilities version 1.8 had to be modified to enable it to process the new WIMS-AECL TAPE16 files generated from the WIMS 3.1 calculations. Moreover, in order to process the WIMS-AECL 3.1 multicell calculations, a new utility had to be developed: RMCELL. This utility program allows the treatment of heterogeneity in the reactor core for the checkerboard pattern and for the fuel and reflector interface.

WIMS Utilities version 2.0 was designed to address deficiencies in version 1.8, and to incorporate user suggestions and improvements. Released in 2008 January, WIMS Utilities version 2.0 is the new consolidated version of WIMS Utilities, computer-platform independent and WIMS-version independent. It supports current and previous versions of WIMS-AECL from version 2.5d, which is the IST version, to version 3.1. It can be run on the HP-UNIX, the PC Windows, and the Shiraz LINUX platforms. Among its many features, WIMS Utilities 2.0:

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- addresses the qualification gaps identified in the configuration management of WIMS Utilities – for example, the utility version label, along with the full configuration details of WIMS Utilities is printed in the output for each major FORTRAN utility;
- corrects all bugs and deficiencies identified in the WIMS Utilities version 1.8 and earlier; and
- updates the four FORTRAN utilities with new features needed for various applications.

Three new FORTRAN utilities were also added to WIMS Utilities:

1. GEN_WIMS Creates WIMS input files for the generation of the WIMS grid-based table, SCM fuel/reflector tables, and micro-depletion fuel/reflector tables.
2. KINPAR Processes two-energy-group cell-averaged cross sections and isotopic reactions, saved on an input TAPE16 file, to generate core-average neutron velocities and the kinetics-parameter table for use in RFSP-IST.
3. RMCELL Processes either DRAGON (Reference [3]) results saved on the CPO file, or WIMS-AECL results saved on the TAPE16 file (Reference [6]) to create the multicell fuel table for use in RFSP-IST.

3.2. WIMS Utilities 2.0 Qualification

Significant changes have been implemented in the four legacy FORTRAN utilities (WRFSP, CONDENS, REGAV, and MICROBURN) since 1999 March. In addition, three new FORTRAN utilities (KINPAR, RMCELL, GEN_WIMS) have been developed. Whether the individual utilities were legacy or new, qualification for the suite of utilities was mandatory.

The AECL SQA Manual requires the following documents for “design and development” of new programs:

- Problem Definition,
- Development Plan,
- Qualification Plan,
- Requirements Specification,
- Theoretical Background,
- Design Description,
- Programmer’s Manual, and
- Verification Reports for the Requirements Specification, Theoretical Background, Design Description, test cases and coding.

These design and development documents were rolled into one document, which was issued in 2008.

The AECL SQA Manual also mandates the following “application” documents for both new and legacy codes.

- Computer Program Abstract,
- Theory Manual,
- User’s Manual, and
- Version Tracking Record.

These application documents have been written for WIMS Utilities version 2.0 and include sections on the four legacy utilities (CONDENS, MICROBURN, REGAV, WRFSP), the three new utilities (GEN_WIMS, KINPAR, RMCELL), and the two PERL scripts (PROC16 and GEN_SIMP). In 2008 January, a fully qualified version of WIMS Utilities, version 2.0 was approved for use.

4. Conclusion

WIMS Utilities version 2.0 is the new consolidated version of WIMS Utilities. Computer-platform independent, WIMS Utilities version 2.0 can be run on the HP-UNIX, the PC Windows, and the Shiraz LINUX platforms. WIMS-version independent, the program supports current and previous versions of WIMS-AECL (version 2.5d, which is the IST version, through version 3.1).

WIMS Utilities version 2.0 can be used not only to generate WIMS-AECL single-lattice-cell cross section tables, but also to generate WIMS-AECL multicell cross section tables from WIMS-AECL TAPE16 files calculated with WIMS-AECL.

The bugs and deficiencies identified in earlier versions and described above, have been corrected. The required SQA documentation – i.e., the design and development documentation, together with the application documentation – for the seven FORTRAN utilities (four old utilities, CONDENS, MICROBURN, REGAV, WRFSP, and three new utilities, (GEN_WIMS, KINPAR, RMCELL) and the two PERL scripts (PROC16 and GEN_SIMP) are in place.

WIMS Utilities version 2.0 is qualified for use in safety analysis, licensing, and routine operation, and is now a candidate to become a reactor physics IST code for the Canadian nuclear industry.

5. References

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