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CURRENT STATUS OF THE GLASS CODE (U)

by

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ABSTRACT

This paper summarizes the current status of the Generalized Lattice Analysis Sub-System (GLASS) computer code[1] and its supporting cross section libraries. GLASS was developed at the Savannah River Site (SRS) in the early 1970's. The GLASS code has been instrumental in supporting safe Heavy Water Reactor (HWR) operations and predicting material production at SRS for more than 20 years. The Department of Energy Office of New Production Reactors (ONPR) program has chosen to use the GLASS code for the design of the HWR option of the New Production Reactor (NPR). A substantial body of validation calculations have been performed and additional validation calculations will be performed to qualify the new GLASS multigroup cross section libraries derived from the ENDF/B-5 and 6 nuclear data files. Several improvements to the code are in progress. Many other improvements are planned to bring GLASS up to modern physics and computer technology.

INTRODUCTION

GLASS is a thermal reactor physics code for computing multigroup neutron and photon fluxes and reaction rates in a two-dimensional lattice of hexagonal or square cells. The photon fluxes are used to estimate gamma heating. Both deterministic (collision and transmission probability) and stochastic (Monte Carlo) methods are used. The deterministic methods are used to compute basic reaction rates and reactivity coefficients, while the Monte Carlo method is used to evaluate the approximations used in the deterministic calculations. Depletion calculations provide estimates of the isotopic composition of the lattice with time. Sets of few-group cell-averaged neutron cross sections are produced for input to the nodal diffusion theory codes used for the steady-state and transient analysis of the SRS reactors. A simple steady-state thermal-hydraulics calculation provides temperature and density profiles in a multi-tube assembly. Therefore, GLASS provides most of the basic information used for the design and operation of the SRS production reactors.

HISTORY

GLASS is a collection of modules which are part of the JOSHUA System developed at the SRS. GLASS was developed during the period 1967-1975 as an extension of the thermal reactor methodology used in the THERMOS[2] and HAMMER[3] codes. Over 25 man-years of effort were expended in the development of GLASS. Because of the limited storage (about 0.5 Megabytes) available in the computers of that period, GLASS had to be divided into many small modules that shared data via disk storage. In addition, linked-list coding techniques were used to manage main storage. As a result, GLASS modules were difficult to program and have been difficult to maintain.

The accuracy and applicability to HWR charges has been generally good, although some "fine-tuning" (e.g., by making cross section changes) has been employed in the past primarily to address U-238 resonance capture effects in low-enrichment Uranium assemblies. Therefore, only minor improvements have been made since 1975 (e.g., implementation of a restart option). In the period 1985-86, GLASS was converted to FORTRAN 77 and a VAX version was made available for off-site use in 1987. Recent interest in the design of a new HWR version of the NPR has led to physics improvements in GLASS by both SRS and Argonne National Laboratory (ANL). A UNIX version of GLASS has been implemented by both Babcock and Wilcox (B&W) and SRS. A complete conversion of GLASS to modern programming and physics standards is currently being planned.

DESCRIPTION OF GLASS

The physics methods implemented in GLASS can be divided into five major areas; resonance capture, multigroup lattice calculations, finite reactor leakage, isotope depletion, and photon transport. The current status and expected improvements in each of these areas will be briefly described in the following sections.

Resonance Capture

The standard resonance calculation in GLASS module CREEP is an extension of the Nordheim integral treatment for two-component lattices[4] to a uniform lattice of multi-tube assemblies. An assembly is modeled using collision probability matrices computed by the cosine currents method[5] for one-dimensional multi-region annular geometry. The Nordheim method uses only isolated single-level Breit-Wigner (SLBW) resonance parameters as were contained in ENDF/B-4 and earlier data file versions.

More accurate resonance representations are used in ENDF/B-5 and 6 and require a more advanced treatment. ANL is developing a new resonance capture module named GLASS-MARIA which uses a multi-annular-region rational approximation and all of the ENDF/B-5 and 6 resonance representations. This module is expected to be available in late 1991.

A new code named MARJORI[6] has been developed at SRS to remove many of the restrictions of the CREEP module. The spatial distribution of the flux is computed using collision probabilities in one-dimensional multi-region annular geometry using either the direct-integration or cosine-currents methods. The energy distribution of the flux and cross sections is essentially continuous. The NJOY[7] code is used to convert (and Doppler broaden) the resonance representations contained on ENDF/B-5 and 6 data files and prepare files of cross sections on a sufficiently fine energy mesh so that linear interpolation can be used to obtain accurate cross sections at any energy. The union of these energy meshes for all isotopes used in a cell defines the energy mesh used in MARJORI. Therefore, resonance overlap and resonance scattering are completely described. The results of the resonance calculation are output in the form of the resonance integrals used by GLASS. Future improvements to MARJORI will also provide for effective resonance multigroup cross sections. It is expected that MARJORI will be available in early 1992.

Lattice Multigroup Calculations

GLASS computes the multigroup neutron flux in a two-dimensional lattice of fuel, target, and control assemblies. The basic geometric unit is a hexagonal or square cell containing moderator and a multi-tube annular or cluster assembly. Cells can be grouped into larger units called supercells. A typical SRS supercell consists of one control assembly surrounded by six fuel and/or target assemblies. The supercell is assumed to repeat by translation and rotation to fill all of space and thus form an infinite lattice of supercells.

A cell is subdivided into regions. A region contains a homogeneous material and is subdivided in subregions. A subregion is a two-dimensional area bounded by sides which are either straight lines or circular arcs. Although GLASS can treat these general subregions, the GLASS input processor restricts the geometry to those types of subregions encountered in typical SRS lattices. The average neutron flux in each subregion is computed by one of several approximations to the multigroup neutron transport equation; the integral transport (collision probability) method, the transmission probability method, and the Monte Carlo method.

The integral transport method is the standard method used in GLASS. Scattering is assumed to be isotropic and the transport approximation is used to correct for P_1 scattering. Any future upgrade to GLASS would remove this restriction and provide rigorous treatment of at least P_1 scattering. Cells are divided into an inner and outer zone. Subregions within a zone are coupled together using collision probability matrices. A Monte Carlo geometry subroutine is used to determine the tracks of neutrons which are then used to compute the collision probabilities. A similar technique is also used in the ANL collision probability code GTRAN2[8]. Zones are coupled together using the cosine currents (DP_0) approximation. This approximation was required by the storage restrictions of the 1970's. It has been tested using the Monte Carlo method and found to introduce little error. However, it is not required today and would be removed in any future version of GLASS. Cells in a supercell are coupled together using the cosine currents (DP_0) approximation. This approximation has been extensively tested using the Monte Carlo method and is quite accurate since the approximation is used in the middle of the large heavy water moderator regions where it is expected to be most accurate. The approximation is essential to reducing the size of the transport matrix by decoupling the matrix into smaller weakly coupled matrices. This allows problems with a large number of subregions to be done without the need for very large storage or virtual memory. Any future version of GLASS would retain this approximation but would probably improve it to at least DP_1.

The transmission probability method assumes a DP_n flux on each surface of a subregion. Transmission probabilities relate the outward-directed angular components of the neutron current with the inward-directed components. The angular components of the currents are then iterated to obtain a solution. Up to DP_3 components can be used. The method has given good results with modest storage requirements. However, it is slower than the collision probability method because of extensive iteration time. More research is required to make this method practical.

The multigroup Monte Carlo method was implemented to evaluate the approximations (P_1 scattering, flat flux, and cosine currents) used in the integral transport method. The method uses the same multigroup data (including the resonance integrals) used by the integral transport method. The Monte Carlo code can either simulate each of the above approximations or not make the approximation.

Finally, any of the above methods can be used to compute the response matrix of a cell. The response matrix relates the components of currents leaving an isolated cell to a unit component of a current entering the cell. The components of these currents generally have 4 groups, 1 or 2 (DP_0 or QP_0) angular components, and 1 or 2 subdivisions of each face of a cell. If a response matrix is computed for each different type of cell in a reactor, then the interface currents can be computed by iteration to solve for the few-group transport theory flux in an entire two-dimensional reactor. The accuracy of the method is limited by the angular and spatial subdivision of the cell face compared to the gradient of the flux along the face. Cells near the edge of a reactor require a much finer subdivision than the 1 or 2 angular and 1 or 2 spatial subdivisions than can be currently computed. Therefore, the method has been rarely used. Increasing the angular and spatial subdivisions in a future version of GLASS will make the response method accurate and practical for large regions of the reactor with many cells.

Multigroup Libraries

The standard GLASS multigroup library uses 54 epithermal groups and 30 thermal groups for a total of 84 groups. The thermal cutoff is at 0.785 eV. The library is a mixture of pre-ENDF/B evaluations along with selected evaluations from ENDF/B-3 through 5. The cross sections for most important nuclides were derived from ENDF/B-4; known exceptions to this are (a) the U-238 resonance parameters are an adjusted set unique to SRS, (b) the U-235 ν (neutrons per fission) data have been revised upward to be consistent with ENDF/B-5, and (c)

the D_2O and H_2O scattering kernels apparently predate ENDF/B-3. The nuclear data in the standard GLASS library have been adjusted to give better agreement with integral experiments and operating data, to correct for errors in the nuclear data, to correct for errors resulting from approximations in GLASS, and to correct for errors in the integral experiments and operating data. This procedure has resulted in a combination of nuclear data and a computer code that is validated in the sense that, together, they successfully predicted the HWR experimental observations at SRS.

While the knowledge of basic nuclear cross sections has continued to expand since the GLASS standard library data was first formulated using ENDF/B-3 and 4, there was no mechanism for GLASS to use the more elaborate resonance formalisms now incorporated in ENDF/B-5 and 6. In order to provide GLASS with access to the latest ENDF/B cross sections, SRS has developed an interface code named WINDEX[9] which takes the output from the Los Alamos National Laboratory (LANL) cross section processing code NJOY and converts them to the GLASS multigroup format. This provides GLASS with access to the latest ENDF/B data, and relieves SRS of the burden of maintaining the cross section processing code. WINDEX also provides the interface between NJOY and MARJORI.

When new ENDF/B-5 libraries were prepared and used in GLASS, the results for H_20 (but not D_20) were found to be sensitive to the thermal upscattering cutoff energy. The standard GLASS library uses a cutoff of 0.785 eV. The initial results obtained from GLASS using the ENDF/B-5 data with 30 thermal groups and an upscattering cutoff of 0.785 eV were not in satisfactory agreement with those obtained from VIM and MCNP using the same ENDF/B-5 data. A 60-thermal group GLASS calculation using the same upscattering cutoff produced essentially the same results as the 30-group calculation. Additional calculations were done varying the upscattering cutoff energy using the standard GLASS energy group structure. In addition to the standard cutoff of 0.785 eV (30 thermal groups), calculations were done at a cutoff of 1.86 eV (34 thermal groups) and 3.06 eV (36 thermal groups). It was necessary to raise this cutoff to over 3 eV to obtain results for H_20 consistent with those from VIM and MCNP which use cutoffs of about 10 eV. Future GLASS libraries will probably use this higher cutoff of 3.0 eV. With these changes, the thermal neutron spectra predicted by GLASS agree well with those predicted by VIM and MCNP. This does not imply that these kernels are an improvement over the kernels previously used in GLASS. Comparison of integral parameters of the kernels (diffusion lengths, cooling coefficients, etc.) with measured values indicate that the ENDF/B-5 kernels may be somewhat improved for D_20 but are worse for H_20. This is a matter of further investigation for future versions of ENDF/B.

Finite Reactor Leakage

The spectrum in a finite reactor is different than the spectrum in the infinite lattice assumed in the lattice flux calculation because there is a preferential leakage of fast neutrons. This change in spectrum is estimated using a Fourier Transform method (also called the B_L method) as first used in MUFT[10]. The detailed space-energy flux in the lattice is used to homogenize the lattice preserving all reaction rates. The homogenized cross sections are then used in a B_L calculation with a predefined amount of leakage (Buckling) or in a variety of searches for a critical Buckling, concentration, or time absorption. The ratio of the homogeneous flux with leakage to that without leakage is used as a correction factor for the lattice space-energy flux. This part of GLASS is quite satisfactory and few changes are anticipated.

The leakage corrected flux is then edited down to few-group cross sections for use in nodal diffusion theory calculations of the full reactor. ANL has prepared a module named GLASS-NET(11) that also edits the inter-cell neutron currents used to compute flux discontinuity factors. A future version of GLASS is expected to have more extensive editing facilities under control of the user.

Isotope Depletion

A control program will step through GLASS calculations to predict the isotopic depletion with time. At each time step a full GLASS calculation is done for the current isotopic compositions. The compositions are then advanced to the end of a depletion time step using the ENDF/B-3 data for reaction rates, fission product yields, decay chains, branching ratios, etc. All of these data are stored in the GLASS multigroup library. Fission products can be treated individually or lumped into long-, medium-, and short-lived products. At each time step the supercell can be maintained critical by adjusting the capture rate in the control cell which simulates the manner in which the SRS reactors are operated.

For the most part, the depletion calculation in GLASS is very satisfactory. However, new multigroup libraries are being prepared from ENDF/B-5 and 6 using NJOY and WINDEX.

Photon Transport

Photon production, photon interaction, and heat generation cross sections derived from ENDF/B-3 are also stored on the multigroup library. The photon production cross sections are used along with the lattice space-energy flux to estimate photon sources in the supercell. These sources are used in a photon

transport calculation (generally using the collision probability method) to estimate the multigroup photon flux in the supercell. The photon energy deposition plus the neutron energy deposition is added to the fission energy deposition to obtain the complete set of heat sources in the lattice.

The improvements described above for the neutron transport calculations will apply to the photon transport calculations (since they use the same coding). This will eliminate the present isotropic scattering restriction which is a poor approximation for photons. In addition, new multigroup photon libraries will be prepared from ENDF/B-5 and 6 using NJOY and WINDEX.

VERIFICATION and VALIDATION

Verification is a demonstration that a computer code solves the problem that it is intended to solve. Validation is a demonstration that the problem to be solved represents physical reality and that the code predicts quantities which are observed. GLASS was verified when it was first developed and when subsequent modifications were made. There is currently a formal V&V documentation in progress for GLASS at SRS and for export versions. The SRS code certification process is nearing completion.

The traditional method of technical validation is to prepare libraries of nuclear data for the reactor design codes and use the codes to predict quantities measured in both clean integral experiments and actual reactor operations. This approach works if the predictions agree within the experimental error, if the measurement error is sufficiently small, and if the scope of the measurements cover the areas of critical design concern.

Difficulties in Validation

It is difficult to validate codes in this traditional manner when the experimental errors are large and lead to comparable design uncertainties. This is the situation with many of the available HWR related physics measurements of highly enriched uranium tritium producing lattices as a result of the uncertainties in the absolute Li-6 content in the tritium producing target tubes used in both experiments and production reactor measurements. Uncertainties in the absolute Li-6 contents do not hinder the safe operation of HWR charges because their composition relative to calibrated standards can be measured to better than 1%. The target tubes are matched relative to the standard so that each HWR charge is very uniform in composition. It is the uncertainties in the absolute Li-6 content of the calibrated standards that make it difficult to validate current lattice reactivity calculations with past measurements of tritium producing lattices.

The NPR program would benefit if the content of the Li-6 calibrated standards were resolved and the measurements reanalyzed. However, even if the content were known to 1%, there are few integral parameters that could be measured that would improve the calculation. The integral parameters that would increase our confidence are temperature, density, and substitution coefficients. Unfortunately, these coefficients are difficult to measure to a precision that would increase confidence in predictive calculations.

A Reactor Physics Technical Working Group (RPTWG) was employed from July 1989 to February 1991 under the direction of ONPR to assess current HWR physics code capability. This working group consisted of one member each from Argonne, Brookhaven, and Sandia National Laboratories, and SRS plus consultants appointed by ONPR. A conclusion reached by the RPTWG was that further critical reactor experiments would not lead to significant improvements in HWR reactor physics. They also noted that increased reliance on controlled numerical "experiments" employing continuous energy Monte Carlo codes would be necessary to validate production codes and define uncertainties in core parameters that cannot be directly measured.

Validation Using Continuous-Energy Monte Carlo Codes

The RPTWG effort centered on validation of the GLASS code by comparison to two Monte Carlo codes; VIM and MCNP. Comparisons were made for five different SRS cold-clean production lattices as well as for effects of temperature, coolant and moderator voiding, and light water addition in a tritium producing lattice. VIM and MCNP solutions were compared to GLASS integral transport and Monte Carlo solutions for the five different production lattices.

The use of two completely independently developed Monte Carlo codes and cross section preparation codes, such as VIM with MC^2, and MCNP with NJOY, both using the ENDF/B-5 library, allowed definition of the precision of cell calculations as well as how an approximation method such as GLASS integral transport compares with more rigorous Monte Carlo. The thermal reaction cross sections for the isotopes in the lattice are well-known having uncertainties less than 1%. When these cross sections are folded together to produce reaction rates in an NPR type of fuel/target assembly, the uncertainties in relative capture and fission reaction rates due to cross sections are well below 1%. It is rare that reaction rates in lattice critical or subcritical assemblies can be measured to this precision.

Eigenvalue Comparisons

The comparison of the two Monte Carlo code results is thought to provide a sufficient basis of precision and accuracy upon which to measure the acceptability of GLASS calculations when all three codes are used to calculate the five SRS production lattice test problems. The cell calculation comparisons were performed for the following HWR lattices: Mark 22 cell and supercell, NPR-80% and 55% cell Mark 15 cell, and the Mark 16-31 supercell. Here, "cell" denotes an infinite array of the specified assembly type while "supercell" denotes a repeating cluster of seven assemblies in which the central assembly is a control assembly and the surrounding assemblies are either six fuel assemblies (as in the Mk 22 supercell) or an alternation of three fuel and three target assemblies (for the Mk16-31 mixed-lattice supercell).

The Mk 22, NPR-80%, and NPR-55% lattices are tritium producing lattices with aluminum clad U-Al fuel tubes and Li-Al inner and outer target tubes. The Mk 22 assembly contains two fuel tubes with a U-235 enrichment of 80%. The two NPR cells have a common geometry (three fuel tubes) but differ in fuel U-235 enrichment (80% and 55%) and in the U-236/U-235 ratio (0.17 and 0.5 for the NPR-80% and NPR-55% cases, respectively). The Mk 15 and Mk 16-31 lattices are plutonium production lattices, with the Mk 15 being a slightly enriched (1.1% U-235) uniform lattice and the Mk 16-31 being a mixed lattice supercell consisting of Mk 16 (60% U-235) driver assemblies and Mk 31 (depleted U) target assemblies. In each case, the fuel and target compositions simulate unirradiated material.

Two-dimensional criticality calculations were performed for infinite (zero-leakage) representations of the various lattices. A uniform temperature of 300K was specified in all cases. The GLASS calculations were performed at SRS using the integral transport option and the standard 84-group multigroup library. GLASS solutions were also obtained using the multigroup Monte Carlo option and same multigroup data in an attempt to isolate errors attributable to the integral transport approximation from those attributable to the GLASS multigroup data. The VIM and MCNP calculations, performed at ANL and SRS, respectively, utilized continuous energy cross section representations derived independently from the ENDF/B-5.2 nuclear data files. Table 1 below illustrates the degree of agreement in lattice eigenvalue, k_∞, between the two Monte Carlo calculations and the GLASS integral transport calculation..

Table 1 Lattice Multiplication, k_∞, Comparison

Lattice	GLASS (Diff)[a]	VIM (1σ,%)	MCNP (1σ,%)
Mk 22 Cell	1.12054 (-0.02%)	1.12072 (0.18)	1.12232 (0.12)
Mk 22 Supercell	1.06817 (+0.04%)	1.06772 (0.23)	
Mk 15 Cell	1.10809 (+1.06%)	1.09636 (0.15)	1.08879 (0.08)
Mk 16-31 SuperCell	0.99690 (-0.01%)	0.99699 (0.29)	
NPR-80% Cell	1.05934 (+0.04%)	1.05890 (0.19)	1.06848 (0.15)
NPR-55% Cell	1.03251 (-0.40%)	1.03659 (0.18)	1.04797 (0.14)

[a] Percent difference between GLASS and VIM results.

An ENDF/B-5 multigroup library for GLASS was generated using NJOY and WINDEX as described above. An exception was the resonance parameters for U-238 and U-236 which were not replaced (GLASS cannot handle non-SLBW parameters). The subsequent GLASS calculations using this library showed that the previous differences observed between GLASS and the Monte Carlo codes were primarily due to the use of different ENDF/B libraries. The results also show that the GLASS code reaction rates come into better agreement with the exception of U-238 absorption. It is expected that the U-238 problem will be resolved when MARJORI is fully interfaced to GLASS.

Reactivity Comparisons

Since changes in reactivity with temperature and density are small, they are very difficult to predict using the statistical Monte Carlo method. These changes are often difficult to measure and few good measurements exist. The designer relies heavily on the deterministic methods built into the production codes such as GLASS. To test the ability of GLASS to predict these small reactivity changes, it was necessary to run the Monte Carlo code VIM for millions (typically 10 million) of neutron histories. The GLASS results shown in Table 2 were obtained at SRS. The VIM results were obtained at ANL.

GLASS using the standard library predicts all of these changes quite well except for the substitution of light water for heavy water (as would occur when the ECCS is used). Note that GLASS predicts a positive reactivity while VIM predicts a negative reactivity.

Table 2 Reactivity Changes for a Mk22 Lattice in pcm (1 pcm (percent milli-k) = 10^{-5} in k)

Change	GLASS	VIM ± 1σ
Coolant Voided	-587	-624 ± 73
Coolant H_2O Substitution	530	-1260 ± 83
Moderator Voided 10%	-391	-374 ± 71
Moderator Voided 20%	-835	-861 ± 72
Moderator Voided 30%	-1340	-1317 ± 73
Fuel Doppler	-103	-93 ± 30
Fuel Doppler + Expansion	-81	-91 ± 31
Target Expansion	-10	-36 ± 29
Coolant Temperature	-203	-164 ± 29
Prompt Temperature Effect	-299	-253 ± 29
Moderator Temperature	-349	-336 ± 26

The replacement of light water for heavy water introduces two effects which tend to cancel. Hydrogen is a stronger absorber than deuterium (a negative effect) but is a better moderator (a positive effect). The effect is sensitive to the thermal neutron scattering kernel used. The GLASS library uses a rather old (pre-ENDF/B-3) version while VIM uses the ENDF/B-5 version. New GLASS calculations with the ENDF/B-5 scattering kernels show greatly improved (and negative) values for the light water coolant substitution case.

Validation of VIM and MCNP

The strategy adopted for the validation of GLASS involves comparison of calculations to the Monte Carlo codes VIM and MCNP. Since these Monte Carlo codes had not yet been validated by NPR QA, an effort was made to sufficiently validate VIM and MCNP to provide a basis for the GLASS validation. The first step was to benchmark the Monte Carlo codes against the Mark 15 LTR-IIA experiment. The results were generally in good agreement with the experimental results except for the MCNP eiger value. A separate unit cell comparison between VIM and MCNP suggests a significant discrepancy in unresolved U-238 resonance capture. To provide a broader basis for validation, members of the RPTWG suggested using available simple geometry critical measurements as a basis for demonstrating Monte Carlo code agreement and accuracy. Six measurements were chosen from the open literature, and the Monte Carlo results agreed very well with all of these experiments.

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