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GRIMHZ VERIFICATION AND VALIDATION SUMMARY REPORT (U)

by E. F. Trumble

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PASTE

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GRIMHX Verification and Validation Summary Report (U)

by

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**GRIMHX Verification and Validation
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1.0 INTRODUCTION

As part of the software quality assurance requirements, the reactor analyses codes used for the calculation of key reactor operating and safety parameters require formal verification and validation (Toffer et al., 1989). The GRIMHX code is used in such applications. Previous documentation exists (Trumble, 1990) discussing the verification and validation of GRIMHX, this document summarizes the past efforts in this area and combines them with recent new analyses performed by WSRC and Westinghouse Hanford Company (WHC). As such, this document is the most up-to-date compilation of verification and validation information pertaining to the GRIMHX code.

The new validation work emphasized two separate features. The first concerned validation of GRIMHX using GLASS produced cross sections for a variety of reactor operating conditions such as shutdown, critical, and at power operation. Different rod withdrawals, fuel loadings, and temperature conditions are considered. Where possible, results are compared to an extensive set of operating data. Otherwise, comparison calculations were performed with the MCNP code.

As shown in Table 1.1, GRIMHX is used to model three different reactor states; shutdown, critical, and power and to account for three types of material property changes; fuel, moderator, and control material. This document validates the use of GRIMHX for these applications through a series of validation problems. Each problem covers a region of the GRIMHX operating envelope. When taken together, these problems provide a complete validation test of GRIMHX over its operating envelope. Therefore, for all calculations falling within this established envelope GRIMHX is considered verified and validated. Using GRIMHX for calculations outside the range tested requires additional validation.

The second feature explored was code validation independent of the GLASS code. Many of the code features such as mesh points, determination of convergence criteria, and core symmetry selections were explored. The new validation effort emphasized matching both the k-effective values and three-dimensional flux distributions against selected benchmark problems.

Table 1.1. Validation Case Matrix

<u>Case</u>	<u>Rx. State</u>	<u>Property changed</u>	
Fuel Chargeback	shutdown	fuel	control rods
K-13 Critical Rod Position	critical	fuel	moderator control rods
Safety Rod Worth	critical	safety rods	
Rod Withdrawal	critical	control rods	
Loss of Fuel Accident	critical	fuel	moderator
K-13 Beginning of Sub-cycle	power	fuel	moderator control rods
K-13 End of Sub-cycle	power	fuel	moderator control rods

This document is organized to present a discussion on verification, validation against experiments, validation against MCNP, and finally validation against operating data. Furthermore, evolution of GRIMHX is considered and its impact on validation results are discussed.

2.0 SUMMARY

The benchmark and operating reactor data analysis with GLASS/GRIMHX represents a significant and unique contribution to the overall verification and validation effort for the two codes. These analyses were independently reviewed and complete records of input and output files were documented. Generally, k-effective comparisons between GRIMHX, MCNP and the ANL benchmark problems were good. A consistent bias was computed between the measured and calculated k-effective for operating data; such biases have been observed in the past.

Extensive matching of three-dimensional flux distributions were performed. For the ANL benchmark problems, excellent agreement was achieved. Radial flux matches with measured data for the K13.1 charge ranged from good to satisfactory. Axial flux profiles were significantly different between GRIMHX and measured data. However, the axial fluxes calculated by ULTRASIM and MCNP agreed with GRIMHX. This points to possible deficiencies in the core model rather than any shortcomings in the codes.

3.0 VERIFICATION AND VALIDATION

Only limited documentation is available that describes the verification of the GRIMHX code during its design, implementation, or testing stages. Therefore, verification is established by comparing the code results against a series of benchmark calculations. These comparison calculations test the different functions of the code and provide assurance that the original configuration of the code was assembled properly and that the different modules of the code interact as expected. Validation of the code focuses mainly on calculations pertaining to the SRS reactors and are either direct comparisons to experimental or measured data or parallel computations performed with the Monte Carlo code MCNP.

3.1 VERIFICATION WITH BENCHMARKS

3.1.1 HTGR Benchmark

In an earlier validation and verification summary (Trumble, 1990), the results of a multigroup hexagonal diffusion theory benchmark solved using GRIMHX were reported. This benchmark, defined in the "National Energy Software Center Benchmark Problem" set (ANL, 1985) contains a solution of a two-dimensional HTGR problem solution, ID.9-A1-2, using GRIMHX. This solution provides verification that GRIMHX solves the two-dimensional hexagonal geometry problem for 1, 3, and 6 points per hex in both standard and coarse mesh and thereby provides assurance about correctness of the computer coding. Both the eigenvalue and group fluxes were compared for the benchmark and both compared very well with the other diffusion theory solutions.

3.1.2 SNR-300 Benchmark

As the earlier benchmark comparisons were done for two dimensions, a need was recognized for a three-dimensional verification for GRIMHX. This was accomplished by selecting a benchmark problem from the "National Energy Software Center Benchmark Problem" set (ANL, 1985). It provided a verification of GRIMHX independent of GLASS cross section generation, since the cross sections were given as part of the benchmark problem.

The benchmark problem is the LMFBR Static Neutronics Problem (ID.18), described on page 794 of ANL (1985). This problem evolved from the MARK I core design of the SNR 300 with some modifications made to the number of materials and geometry to reduce the complexity of the problem.

Table 3.1 shows the eigenvalues calculated by GRIMHX fall within the range of the published solutions (format is problem#, solution type#, solution#, e.g. 18-A1-1). The last value for each solution has the largest number of mesh spaces, and thus is expected to be the most accurate. The region average fluxes were compared with one of the published solutions (Erickson, 1991b), and were found to be typically within 1% to 2% of the published values except for the outer blanket region. GRIMHX is limited to certain numbers of hexagonal assemblies because it requires full patches (a patch is a group of seven assemblies). The GRIMHX model of the benchmark problem required additional assemblies outside the radial blanket to form complete patches. With these additional assemblies, the flux is not exactly zero on the outer boundary of the radial blanket. This slightly increases the flux level in the radial blanket and accounts for the 10% error in the region. The 5% to 10% differences in the outer rod region occurs in a region where the absolute flux levels are 500 times smaller than the peak flux. Overall, GRIMHX did an excellent job of reproducing both the eigenvalues and the region averaged fluxes. This shows GRIMHX's ability to correctly predict reactivity and flux distributions in three dimensions for multigroup, hexagonal geometries.

3.2 VALIDATION - EXPERIMENTS

In 1974 a series of two-dimensional space- and time-dependent experiments were performed to test the transient version of the GRIMHX code - TRIMHX (Trumble, 1990). GRIMHX was used to calculate the asymptotic solution to local perturbations. GRIMHX was employed to compute the flux tilts and the reactivity addition to the lattice in question. The absolute flux tilts were calculated to better than 5%. The reactivity addition calculated by GRIMHX matched the measured results exactly. Although these experiments were designed to measure time-dependent phenomena, useful validation of the GRIMHX code was achieved.

In 1977, Similar applications of GRIMHX to three-dimensional space-time measurements were carried out (Trumble, 1990). Again, GRIMHX was used to calculate the asymptotic flux levels associated with the perturbation and the size of the reactivity perturbation. The agreements observed in flux tilts were within 5% and reactivity predictions were very close to measured data.

3.3 VALIDATION - MCNP COMPARISONS

3.3.1 Safety Rod Worth

WSRC-RP-89-1248, "Validation of GRIMHX Calculations for Safety Rod Worth, Rev. 1" compares GLASS/GRIMHX and MCNP calculations for a series of nine benchmark calculations used to compute safety rod worths. The objective of the safety rod worth study was to demonstrate confidence in GRIMHX's ability to calculate safety rod worths used in formulating Technical Specifications and accident analysis. GRIMHX calculations used several different radial power shapes to investigate the effect of different radial flux profiles on the safety rod worth.

A comparison of the results from the two codes is shown in Table 3.2. The eigenvalues for GRIMHX and MCNP as well as the delta eigenvalue (i.e. safety rod worth) for the nine cases described in the reference are provided in this table. Uncertainty intervals are given for the MCNP calculations based on the statistics of the calculations. GRIMHX results of $\Delta k/k$ for six of the nine cases fall within a 1σ (sigma) uncertainty of MCNP, while the remaining three are within 2σ . In addition, the MCNP results bracket those of GRIMHX. All the scatter is well within the uncertainty of the statistical nature of the MCNP calculations.

This work provides a good validation of GRIMHX and GLASS for the case of a change in a strong absorber like the safety rods.

3.3.2 Loss of Fuel Accident

The Loss of Fuel Accident (LOFA) involves the melting of a near center fuel assembly with the consequent release of molten debris into the moderator. The

Transport/Diffusion Theory) and MCNP (Monte Carlo transport). A three-dimensional, explicit full-core model of the SRS reactors, developed for the Loss of Fuel Accident (LOFA) study, has been formulated using the MCNP Monte Carlo transport computer code (Breismeister, 1986). The MCNP model (Okafor, 1991d) is used as a benchmark for reactivity worth analysis of the LOFA done with GLASS/GRIMHX.

Two 3-D cases were modeled as part of this validation. The first involved an "ideal" model consisting of a uniform debris concentration in the moderator of a strongly confined area of the core. This simplified version of the accident was used to ascertain the applicability of diffusion theory (GRIMHX) to such a problem. The second model consisted of a time dependent debris distribution axially and radially in the core. In this second model not only was the debris tracked, but the fuel tube melt was accounted for explicitly. Thus perturbations to the fuel position and the bulk moderator were performed.

The homogeneous LOFA runs show good agreement between GRIMHX (Clever, 1991) and MCNP (Okafor and Zino, 1991a). The time-dependent cases agree to within the statistical uncertainty of MCNP (Okafor and Zino, 1991b) as shown in Table 3.3. Both sets of calculations demonstrate the consistency between MCNP and GRIMHX for a complicated scenario involving changes in both the fuel and moderator configuration.

3.3.3 Rod Withdrawal

A series of GRIMHX cases were performed to validate the code for rod withdrawal scenarios. Parallel MCNP calculations (Okafor and Zino, 1991c) were performed for comparison to the GRIMHX calculations. These cases were all at cold, unexposed, beginning-of-life conditions. Both codes were used to calculate rod worths for each rod withdrawal sequence. These calculations are described in the GRIMHX Benchmarking report (Erickson, 1991).

As shown in Table 3.4, GRIMHX predictions of k-effective agree with the MCNP predictions to within a 1σ uncertainty. Due to combinatorial statistics, the worth of the rods for the first case is just outside a 1σ band, but well within 2σ . For the second case, GRIMHX and MCNP calculated control rod worths agree to within 1σ .

3.4 VALIDATION - OPERATING DATA

3.4.1 Fuel Chargeback

Neutron flux monitoring of the fuel chargeback for the L-4 charge was performed using an internal fission counter (IFC). This information provides a benchmark problem for GRIMHX for a subcritical reactor by comparing computer predictions with actual measured results (Bond, 1990).

Predictions of the IFC response during the L-4 chargeback were performed using a three-dimensional GRIMHX reactor model. Cross sections for the reactor model were generated using GLASS. Gang average contents were used for the L-4 Mark 22 charges. Static source calculations were performed using the coarse mesh option with one point per hex and 50 axial points. IFC locations were modeled by leaving the hex position vacant with the thermal flux in the vacant positions used to represent the response of the IFC. The relative IFC response was determined by the initial count rate with only neutron sources (no fuel) in the reactor.

Table 3.5 shows the measured and calculated changes in the relative count rate of the IFC during the L-4 chargeback. GRIMHX over-estimates the measured data, however the error is nearly constant for the higher count rates.

The fact that GRIMHX is predicting a greater count rate than is actually measured is conservative for setting count rate limits during a chargeback. However, for a validation problem, the desire is to demonstrate how faithfully the calculation actually represents a real situation. GRIMHX does a very good job of predicting the trend in the measured data. The GRIMHX predictions fall nearly on top of the measured data when rescaled to match the higher count rates. This can be clearly seen in Figure 3.1. As justification for renormalizing the predictions, the original scale factor was obtained using the observed count rate with no assemblies in the core. Under these conditions of no fissile material, the flux may be more sensitive to the moderator properties than a fully loaded core.

The success of GRIMHX in predicting the chargeback provides a good validation of the code for the sub-critical or shutdown core with less than a full fuel loading and with a static source. Because the chargeback sequence poses a highly space-dependent problem with fixed detector and source locations and a changing core size, this problem provides a good verification of the three-dimensional capability of GRIMHX to model perturbations to fuel positions.

3.4.2 K-13 Initial Critical Rod Position

Three operating conditions for the K13 charge have been modeled using the GRIMHX code with individual assembly types modeled by GLASS. The GLASS macroscopic cross sections were used as input to GRIMHX for the whole core computation. The predicted k-effective values were compared to critical ($k_{eff} = 1.00$) in the GRIMHX Benchmarking report (Erickson, *et al.*, 1991). The first condition modeled was a cold, initial critical case (Startup). In order to further test GRIMHX, the initial critical case was modeled three ways; full core, half core rotational symmetry, and sixth core rotational symmetry. The whole core, half core, and sixth core models produced essentially identical results. As a further test, this case was also modeled with MCNP (Okafor and Zino, 1991d). The k-effective values predicted by GRIMHX (and MCNP) are shown in Table 3.6. As shown, the GRIMHX and MCNP predictions are within 100 pcm for the initial critical case, although they show an almost 2000 pcm bias from critical. Earlier work (Webb, 1988) in modeling nine individual reactor initial critical states showed similar biases. In this work, the mean bias found when comparing calculated criticals to measured was 1500 pcm with a range (at 95% confidence) of between about 1300 and 1700.

3.4.3 K-13 Beginning of Cycle and End of Sub-Cycle

The critical rod positions were also modeled for a BOC case which was shortly after startup and used low exposure fuel. The third critical case, the EOC, was shortly before the mid-cycle shutdown (end of K13.1 sub-cycle) and used moderate exposure fuel. In the BOC case, as in the initial critical, there was an approximately 2000 pcm bias from critical. The EOC case had a bias of approximately 3500 pcm.

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It is likely that the 2000 pcm bias seen in the initial critical and BOC case is a result of uncertainties in the material concentrations. Scoping calculations indicated that a 10.0% reduction in the Li-6 concentration in the outer targets brought the bias down to less than 100 pcm (see Table 3.6) for both the GRIMHX and MCNP models. This same dependency on contents was seen in the earlier work (Webb, 1988). Much of the additional 1500 pcm bias seen in the EOC case may be attributable to oversimplification in the exposure model used, or to the fact that control rod burnup was not accounted for in the modeling.

The results of the GRIMHX calculation of the BOC and EOC models were compared to measured power data, and the BOC case to calculations by other codes, specifically MCNP and ULTRASIM (Gregory, 1989), the reactor simulator code. The measured data consists of a total power for every assembly and interpolated data from the nine axial power monitors (APMs) for both the BOC and EOC cases.

Comparisons were made of the axial data for the initial critical case and of the radial power for both the BOC and EOC cases. GRIMHX calculations produced thermal flux data corresponding to the measured data. ULTRASIM produced gamma and neutron fluxes for the BOC case only. MCNP produced axial thermal flux distributions on a gang average basis for the BOC case only (Erickson, *et al.*, 1991).

The GRIMHX, MCNP and ULTRASIM codes predicted axial power shapes that agree quite well with each other, but fail to reproduce the measured axial data. The general agreement on the axial power profiles between GRIMHX, ULTRASIM, and MCNP suggests that the failure to accurately predict the measured axial data is the result of a weakness in the modeling of the core (which was common to all of the codes) and not in the codes themselves. Further work in refining the models used for the axial shape comparisons are planned to try to bring the GRIMHX calculated reactor response closer to that seen in the measured data. Work is also planned to provide for external initialization of GRIMHX to a specified (measured) set of power shapes.

GRIMHX calculated radial profiles show much better agreement with the measured data, particularly in the BOC case. The differences in the EOC radial distributions between GRIMHX and the measured data may be attributable to oversimplification of the exposure model, or due to the fact that control rod burnup was not accounted for in the EOC model.

4.0 COMPARISON OF PAST AND PRESENT CODE VERSIONS

To establish if any coding changes in GRIMHX had taken place since its inception, a series of test problems were rerun. The results Gregory obtained in 1989 with the latest version of GRIMHX matched the original flux values (1975 study) and eigenvalues to within four significant digits (Trumble, 1990). The conclusion that can be drawn from this is that the code is essentially the same code as the original version and that any of the past verification and validations are still applicable to the present version.

5.0 QUALITY ASSURANCE

This report was generated under QA Task 90-044-1 "Certification Plan for GRIMHX, TRIMHX and GILDA". It fulfills the requirements of the Verification and Validation Plan (Toffer et al., 1989) for GRIMHX. Review and records retention for the new analyses discussed in the report meets quality assurance requirements. All new calculation results are stored in microfiche binders (Trumble, 1990b).

6.0 CONCLUSIONS

The validations and verifications discussed in this report, in conjunction with those described in the earlier V&V Summary Report (Trumble, 1990) validate the GRIMHX code over a wide range of applications. The code has been validated for 2- and 3-D problems, with "standard" and "coarse" mesh, with one or multiple points per hex, under several different reactor symmetry options. The code has also been validated for all three reactor operating states (shutdown, critical, and power) which it is called upon to model. The reactivity worths and flux perturbations due to changes to fuel, control or bulk moderator positions has been shown to compare well to benchmarks, experiments, similar codes and to operating data.

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Table 3.1. Eigenvalue Comparison With other Benchmark Solutions

<u>Benchmark Solutions</u>	<u>mesh</u>	<u>eigenvalue</u>
GRIMHX		
	1x72x22 (coarse)	1.0134
	6x72x22 (std)	1.0140
	6x72x22 (coarse)	1.0128
18-A1-1		
	34x17x18	1.0166
	68x34x36	1.0130
	102x51x54	1.0123
18-A1-3		
	18x18x19	1.008466
	35x35x37	1.012154
	52x52x55	1.012776
18-A1-4		
	18x18x19	1.006753
	35x35x37	1.009964
	52x52x55	1.010660
	extrapolated	1.011050

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**Table 3.2. GRIMHX and MCNP Calculations
of Safety Rod Worth**

<u>Problem number</u>	<u>Rods out</u>	<u>Rods in</u>	<u>delta k</u>	<u>delta k/k (%)</u>
1	0.98084 0.977440 ± 0.0013	0.9500 0.946229 ± 0.0014	0.03084 0.0312 ± 0.0019	3.14 3.19 ± 0.19
2	1.01972 1.022134 ± 0.0014	0.98807 0.990707 ± 0.0013	0.03165 0.0314 ± 0.0019	3.10 3.07 ± 0.19
3	1.01972 1.022134 ± 0.0014	0.99399 0.993686 ± 0.0011	0.02573 0.0284 ± 0.0018	2.52 2.78 ± 0.18
4	1.03021 1.032250 ± 0.0012	0.99746 1.00283 ± 0.0014	0.03275 0.0289 ± 0.0018	3.18 2.85 ± 0.18
5	1.03021 1.032250 ± 0.0012	1.00252 1.004005 ± 0.0017	0.02769 0.0282 ± 0.0021	2.69 2.74 ± 0.21
6	1.01859 1.021089 ± 0.0012	0.986 0.988542 ± 0.0015	0.03259 0.0325 ± 0.0019	3.20 3.19 ± 0.19
7	1.012 1.007901 ± 0.0014	0.97828 0.975266 ± 0.0016	0.03372 0.0326 ± 0.0021	3.33 3.24 ± 0.21
8	1.00415 1.004594 ± 0.0012	0.97253 0.976165 ± 0.0015	0.03162 0.0284 ± 0.0019	3.15 2.83 ± 0.19
9	0.993 0.994148 ± 0.0015	0.96154 0.963479 ± 0.0014	0.03146 0.0307 ± 0.0021	3.17 3.08 ± 0.21

**GRIMHX
MCNP**

Table 3.3. Comparison of GRIMHX and MCNP
for the Time Dependent LOFA

<u>Time (sec)</u>	<u>GRIMHX (pcm)</u>	<u>MCNP (pcm)</u>
1	-76	- 98±156
2	-13	- 54±156
3	38	16±156
4	42	- 93±156
5	2	-118±156

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Table 3.4. Rod Withdrawal Results

	<u>GRIMHX case_id</u>	<u>GRIMHX k-eff</u>	<u>MCNP k-eff</u>
1. 1 rod from each septifoil, Gangs 1, 2 and 3.			
a. 3000-NP (Base Case)	VALDRW1	0.99901	0.9981 ± 0.0012
b. 2000-NP	VALDRW3	1.02337	1.0242 ± 0.0010
	Worth =	2438.4 pcm	2615 ± 157 pcm
2. 2 rods from each septifoil, Gang 1 only.			
a. 3000-NP (Base Case)	VALDRW1	0.99901	0.9981 ± 0.0012
b. 1000-NP	VALD2RW2	1.0168	1.0161 ± 0.0013
	Worth =	1780.8 pcm	1803 ± 177 pcm

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**Table 3.5. Differences Between Measured Data During L-4
Chargeback and GRIMHX Predictions**

Assemblies Loaded	Measured Data (M) IFC (25,63)	Calculated Data (C) IFC (25,63)	Examples of Rescaling Data (0.85*C)
1	1.0	1.0	
3	1.8	2.3 (-22%)	
12	5.6	6.1 (- 9%)	5.2 (7%)
24	13.9	14.2 (- 3%)	12.1 (13%)
47	24.6	25.2 (- 3%)	21.4 (13%)
64	29.6	32.1 (- 8%)	27.3 (8%)
93	35.4	40.2 (-14%)	34.2 (3%)
128	43.4	49.5 (-14%)	42.1 (3%)
170	48.3	56.5 (-17%)	48.0 (1%)
216	53.5	62.3 (-16%)	52.9 (1%)
263	57.9	67.3 (-16%)	57.2 (1%)
323	61.8	71.3 (-15%)	60.6 (2%)
382	64.1	74.2 (-16%)	63.1 (3%)
417	66.4	75.6 (-14%)	64.3 (3%)

Note: The value in parenthesis is the percent difference between the measured value and the calculated value.

Table 3.6. Critical Rod Position Predicted k-eff.

	GRIMHX k-eff	Bias (pcm)	MCNP k-eff	Bias (pcm)
COLD, CLEAN CASES				
Startup (full core)	0.98186	1814.0	0.9809±.0011	1910.0
Startup (half core)	0.98186	1814.0	-----	
Startup (sixth core)	0.98186	1814.0	-----	
10% reduction in Li-6 in outer targets	1.0009	90	0.9995*	50
HOT OPERATING CASES				
BOC K13.1	0.98379	1621.0	-----	
EOC K13.1	0.96540	3460.0	-----	

* extrapolated from K-5 data

Figure 3.1

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9/8/93

END