REBUS-PC v1.5 Verification Test Summary

Nuclear Science & Engineering Division

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September 2019

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Executive Summary

Motivated in part by its usage for analysis of the University of Missouri Research Reactor (MURR), the verification of the REBUS-PC software for θ -R-Z geometries is discussed and displayed in this manuscript. Of particular importance is to show that the eigenvalue, flux, power, and burnup outputs of the software given a user problem is correct. REBUS-PC contains many features and MURR only makes use of some of those aspects. As an example, the use of region specific cross section sets, interpolation of the cross section data with respect to burnup, and automatic movement of control rods during the fuel cycle is discussed and displayed.

To demonstrate the accuracy, 22 verification tests based upon 7 physical geometries are discussed. Geometry descriptions are provided in Section 2 and the REBUS-PC results for each verification test are discussed in Section 3. These verification tests consist of both analytic problems with known solutions and a more complicated input consistent with usage of REBUS-PC on the MURR reactor itself called STRZ. In this verification test summary report, the REBUS-PC software is repeatedly demonstrated to reproduce, or closely match, the eigenvalue, flux, and power distributions from analytic test problem solutions, demonstrating that the implemented finite difference approximation in θ -R-Z is working as intended. Several additional REBUS-PC features are tested, such as control rod movement by detailed comparisons of the results against reference solutions obtained using an auxiliary implemented MatLab program.

As expected, the REBUS-PC software produces results that are 100% consistent with the stated capabilities and thus the verification exercise is completed. These verification tests should be executed with each re-compilation of the REBUS-PC source and after any source code changes. All output results from any such new work should be rigorously compared against the stored output of the 22 verification tests cited in this report that forms the basis of the verification process.

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1 Introduction

The REBUS-PC software [1-3] has been used extensively to model fuel burnup in both thermal and fast spectrum systems. More recently, the REBUS-PC software has been used for reduced enrichment fuel design efforts for the University of Missouri Research Reactor (MURR). As part of the ongoing work on MURR [4-5], the reliability of the results obtained with REBUS-PC must be more rigorously verified and thus this manuscript serves as proof that the embedded algorithms and output obtained from REBUS-PC are correct.

To begin, the parts of REBUS-PC that must be tested with respect to the MURR work must first be identified. This was done previously [6] and the summary of those capabilities is given in Table 1-1.

Table 1-1. REBUS-PC Identified Capabilities that Must be Verified.

Index	Description
1	Properly implemented θ -R-Z geometry modeling of the diffusion equation
2	Define cross section specific (color set) compositions for use in the multi-group diffusion equation in specific regions
3	Depletion is based upon the provided cross section data in specific regions as defined by Capability #2.
4	Properly implemented reflected boundary condition in the R direction
5	Properly implemented extrapolated boundary condition in the R and Z directions
6	Properly implemented internal boundary conditions for control rods (i.e., “black” boundary conditions)
7	Correct integral power output provided on input spatial regions and areas (collections of regions).
8	Properly implemented control rod movement during depletion over a given fuel cycle
9	Properly implemented Z direction mesh refinement in control rod movement algorithm
10	K-effective solution of the forward multi-group diffusion equation using Tchebychev acceleration and up-scattering iterations
11	Proper implementation of the cubic spline interpolation treatment of the cross section data with respect to a reference isotope density.
12	Proper implementation of the linear interpolation treatment of the cross section data with respect to a reference isotope density.
13	Proper generation of TYPE13.BCD auxiliary output files
14	Proper implementation and convergence checking on the region density iteration scheme for solving the Bateman depletion equations (without extrapolation).

These various capabilities are connected, and thus each test case serves as a test of more than one capability. As an example, capability 1 cannot be verified independent of capabilities 2, 4, 5, and 9 or vice-versa. Beyond this, capability 10 cannot be verified without first verifying capabilities 1-5. In this sense, the verification test suite will have to use problems that combine the checking of each capability which, invariably, is some level of duplicate checking.

2 Selection of Verification Test Models

For rigorous testing, a geometric setup in θ -R-Z geometry was created based upon the IAEA Cartesian benchmark for a generic 10 MW reactor [7]. The original 10 MW Cartesian reactor layout is shown in Figure 2-1. The θ -R-Z representation of this benchmark problem is shown in Figure 2-2, which is referred to as STRZ (simple θ -R-Z) in this manuscript.

Figure 2-1. Illustration of Original IAEA Generic 10-MW Reactor Model

Figure 2-2. STRZ Benchmark Problem Geometry Details

From Figure 2-1 one can see that the original core is a 5×6 element core that contains 23 MTR-type standard fuel assemblies and 5 control assemblies. This core is reflected by graphite on two opposite sides and is surrounded by water. One water-filled flux trap is located near the center of the core and

another near the upper left edge. Each fuel assembly consists of 23 fuel plates, and each control assembly consists of 17 fuel plates and 4 Al control plates.

The STRZ problem in Figure 2-2 poses a realistic sized problem consistent with that used in the MURR work and the same input setup is thus used. The STRZ problem preserves the total fuel mass and the fuel to moderator ratio of the original IAEA benchmark problem. From Figure 2-2, the core has four annular rings of fuel each broken into 8 azimuthal regions each separated by water and surrounded overall by two aluminum annular rings. Each fuel region is the same thickness and is composed of a homogenized mixture of fuel meat and cladding. A control blade was placed outside of the core region and is broken into 4 pieces by quadrant, all of which are typically inserted to the same depth. The core is radially surrounded with an annular graphite reflector and water pool, and axially with an upper structure and axial pool region.

The material compositions and multi-group cross section libraries are taken from the IAEA reactor description. For verification purposes, the cycle length is set to one month (30 days) with 10 subintervals. REBUS-PC was used to compute the multiplication factors at the beginning and the end of cycle to be 1.07900 and 0.99859, respectively. Block nuclide depletion is performed for each fuel plate and control blade. Each of the fuel plates is axially divided into three depletion zones with equal heights as shown in Figure 2-2. Four fission products (iodine-135, xenon-135, promethium-149 and samarium-149) and the major actinides (uranium, plutonium and neptunium) are modeled explicitly in the depletion chain. The REBUS-PC input file for this described test case of the STRZ benchmark problem is provided in the source code repository.

Given that the problem defined by Figure 2-2 and its described depletion chain is not analytically solvable, code-to-code comparisons are required or, alternatively, an independent solution of the underlying equations is required as a basis to support accuracy of REBUS-PC. These details are discussed later in this report when providing the calculated results for the STRZ benchmark problem.

In addition to the STRZ verification test, the multi-group diffusion equation can be solved analytically under certain circumstances which provides the best verification base of the steady state neutronics solver in REBUS-PC. In this work, a one-group and seven-group cross section data set is used to validate some of the capabilities in Table 1-1. To systematically verify several of the capabilities, the following benchmark problems were constructed to check the accuracy of the DIF3D finite difference diffusion theory flux solver and depletion capabilities of REBUS-PC.

2.1 One-Group, 1-D Analytical Benchmark

The first test case is a one-group, 1-D cylindrical homogeneous core problem which is named 1GCYL_hom. This benchmark uses a reflected boundary condition at the center and an extrapolated boundary condition at the outer edge of the cylinder. This benchmark problem checks the accuracy of the eigenvalue calculation routine of DIF3D (flux solver of REBUS-PC) and the radial boundary conditions.

2.2 One-Group, 1-D Analytical Benchmark with Internal Black Absorber

The second test case is a one-group, 1-D cylindrical homogeneous core problem named 1GCYL_black. This benchmark has a reflected boundary condition at the center and an extrapolated boundary condition at the outer edge of the cylinder. As can be seen in Figure 2-3, an additional layer of black absorber material is added around the homogeneous region. This benchmark problem checks both

the eigenvalue calculation routine of DIF3D (flux solver of REBUS-PC) and the radial and black boundary conditions.

Figure 2-3. 1GCTL_black Model Showing Black Absorber

2.3 One-Group, 3-D Analytical Benchmark

Unlike the 1GCTL_hom benchmark problem, this problem consists of a single homogeneous region and makes use of radial extrapolated boundary conditions, axial reflected boundary conditions, and periodic boundary conditions in θ to produce an identical solution to 1GCTL_hom. It is named 1GTRZ_hom and uses the same composition as 1GCTL_hom for the core region. This problem can also be used to verify the accuracy of the eigenvalue calculation and the radial, axial, and θ boundary conditions.

2.4 One-Group, 3-D Analytical Benchmark with Internal Black Absorber

This is the 3-D representation of the 1GCTL_black problem. It uses radial extrapolated boundary conditions, axial reflected boundary conditions, and periodic boundary conditions in θ to produce an identical solution to 1GCTL_black and is named 1GTRZ_black. It uses the same compositions as 1GCTL_black and can be used to verify the accuracy of the eigenvalue calculation and the radial, axial, and θ boundary conditions.

2.5 Seven-Group 0-D Analytical Benchmark

In order to test the up-scattering capability listed in capability 10, a simple infinite homogeneous test case was created named 7GTRZ_hom. To test the accuracy of the up-scattering iteration, the cross section data was manipulated to have a significant fraction of up-scattering in the lower energy groups.

2.6 Seven-Group 0-D Depletion Benchmark

To verify the multi-region depletion capability 3, a test problem was constructed of three separate, different sized regions but with equal flux levels named 7GXYZ_hom. A seven-group cross section library is used where identical fuel compositions are assigned to each region. A new utility program was created to serve as an independent calculation of the Bateman (depletion) equations to verify the accuracy of the REBUS-PC solution.

2.7 Seven-Group 3-D Verification Benchmark

The last problem created is a seven-group heterogeneous core problem named 7GTRZ_het. This problem has two different fuel regions surrounded by two reflector regions. A reflected boundary condition is used at the radial center, extrapolated boundary conditions are used at the outer radial edge and both axial surfaces, and periodic boundary conditions are used in the θ direction. The planar view of the configuration is illustrated in Figure 2-4.

Figure 2-4. Configuration of the 7GTRZ_het Model

2.8 Summary Discussion of Verification Test Suite

Table 2-1 shows the set of verification tests constructed for REBUS-PC that are discussed in this report. For each row, the benchmark is named according to the preceding short description, and in some cases the specific purpose is listed. As an example, in verification test #5, 1GTRZ_hom was modified to include reflected boundary conditions on all surfaces to verify capabilities 1, 4, and 5.

In Section 3, input and output excerpts are presented for each verification test listed in Table 2-1. How each problem provides verification of the capabilities listed in Table 1-1 is also discussed. This will involve expanding the description of each capability in Table 1-1 and explaining how a given problem satisfies that aspect of the verification. With regard to the organization of the verification process, independently checking each capability with a single verification test is impractical as the various capabilities are interconnected. As shown in Table 2-1, the focus is placed on discussing each benchmark problem and how it satisfies a given capability rather than creating a list of verification tests that when combined verify a given capability. Thus, as discussed, the set of verification tests are duplicative as the same capability is tested in multiple test problems.

Table 2-1. REBUS-PC Verification Test Suite

Test	Description	Capabilities Verified
1	1GCTL_hom	
2	1GCTL_black	
3	1GTRZ_hom	1, 4, 5
4	1GTRZ_black	1, 6
5	1GTRZ_hom with reflected b.c.s	1, 4, 5
6	7GTRZ_hom	10
7	7GTRZ_hom	10
8	7GTRZ_hom	10
9	7GTRZ_het with fixed source	1
10	7GTRZ_het	1
11	7GTRZ_het using area assignment input	1
12	STRZ with fixed format input	1, 2, 3, 7, 13
13	STRZ with free format input	1, 2
14	STRZ with overlaid geometry	1, 2
15	STRZ with 1W and no CR movement	8, 9
16	Duplicate of Test #19 using A.ISO input	1
17	Duplicate of Test #19 using ISOTXS input	1
18	STRZ with linear spline XS interpolation	3, 12
19	STRZ with cubic spline XS interpolation	3, 11
20	STRZ with polynomial XS interpolation	3
21	1GCTL_hom with modified decay	3, 14
22	7GXYZ_hom	3, 14

3 Verification of Stated Capabilities

The focus of this section is to provide concrete verification of the stated capabilities of REBUS-PC that are used in the MURR work. All of the verification tests are part of the REBUS-PC repository and verification checking system, and were first executed for version 1.5. Each time a source code change is made or a new executable is compiled, the set of verification checks that are described here, along with a selected MURR calculation, are executed to ensure the integrity of the work done here for verification and that done previously on the MURR work itself. In this regard, this work is instrumental in the creation of the first 22 verification tests in the REBUS-PC test suite, where the MURR benchmark can be identified as a verification test named “murr_ne_onestep.” In addition to these tests, the IAEA 10 MW benchmark problem mentioned previously is included in 5 verification tests along with other test cases taken from previous work using REBUS-PC. Combined, these verification tests ensure the integrity of the software as the software, compilers, and operating system progress.

3.1 REBUS-PC Example Input Detail and Relation to Capability Testing

From Table 1-1, several of the capabilities require that various aspects of the user input is checked. To do this, the REBUS-PC input itself, which is broken into several parts: A.STP027, A.SUMMAR, A.DIF3D, A.HMG4C, A.NIP3, A.BURN, and A.ISO or ISOTXS, must be discussed. Combined, these inputs define a problem to be solved using REBUS-PC and specify which outputs are desired by the user. To begin, an example MURR input deck is dissected when describing each segment of the input as it clearly demonstrates the user’s typical input for a given problem. In total, the manual itself should be the ultimate guide for defining the input. The examples presented in this section are for illustration.

3.1.1 A.STP027 Input of REBUS-PC

The A.STP027 input is the control input for REBUS-PC. For the example MURR input it is:

```
UNFORM=A.STP027
01 0 0 0 1 0 0 0 1 0 999999 1
02 0 1 0 2 0 0 0 0 0 1 0
03 0 0 0 1 1 1 0 0 000000 000000
04
05 0 0 1 1
```

As can be seen, the input is wholly a set of integer values. In none of this input are the number of iterations controlled. This input is purely the decision process as to when and what outputs are to be printed during the iterative convergence. In some cases the array memory sizes can be controlled. The only real physics control is the integer flag (0 or 1) that tells REBUS-PC whether an equilibrium or non-equilibrium problem is to be executed, of which, only the latter are relevant for REBUS-PC (the equilibrium solution option is actually physically disabled in REBUS-PC, such that only non-equilibrium problems can be executed).

Given this input constitutes basic control input, it can only be checked by comparing the function of the input and the expected output produced by REBUS-PC. As an example, one of the control flags allows the optional printing of the mass flow table and thus the only check that can be performed for this input is to ensure that the table of data is printed consistently with the provided input.

3.1.2 A.DIF3D Input of REBUS-PC

The next section of input provided to REBUS-PC is the control input for the DIF3D steady state neutronics solver. Similar to the previous case, this input is primarily focused on the memory controls and what outputs are to be produced by the software. In addition, this section of input also controls the iteration limits to be applied in the neutronics solver along with what acceleration to apply and whether up-scattering iterations are to be used. The MURR example input is given as:

```
UNFORM=A.DIF3D
01      Detail MURR 10MW Generic NEQ HEU.UAlx.24PL
02 20      50000      0
03 0 0 0 4500 50 0 0 5 1 0 50
04 1 0 0 00 000 10 000 0 0 0 0
05 1.0-5 1.0-4 1.0-5
06 1.0 1.0-3 4.0-2 12.0+6
```

As can be seen, the input is broken into 6 different card types which is only a subset of the actual card input that is allowed by the software. Card type 01 is a simple title card which does not need to be verified. Card type 02 defines the array memory sizes to apply, which also does not need to be verified. Card type 03 controls the type of acceleration to use, the number of fission source iterations, upscattering iterations, and various other settings which control the behavior of the finite difference solver. Card type 04 controls the output tables that are produced by DIF3D, such as the region-wise and mesh-wise integrated power tables. Card type 05 specifies the desired convergence of the steady state neutronics solution at each time point in the depletion algorithm. Card type 06 specifies constraints on the convergence limits of card type 05 along with the total reactor power (12.0E+6 Watts).

With respect to software verification, the convergence criteria are the first to be discussed, which all have a lower limit of $\sim 10^{-12}$. Verification that the software properly implements these controls is done as part of the analytic solution set of test problems. As is the case for every problem, the analyst is required to verify that the settings are appropriate when they do their validation. Thus the setting for any particular control is problem dependent. For several of the test cases the convergence limit is set to the minimum value possible such that precise answers are obtained. This is sufficient proof that the convergence criteria are being observed by the software. To check the acceleration algorithms, they are disabled and the unaccelerated, fully converged result is compared with the accelerated converged result. This is part of the verification is required for capability 10. Whether or not they pose any improvement in efficiency is not relevant to the software verification purpose of this report. Similarly, the software cannot be verified to explicitly use a given number of upscattering iterations, as this information is not reported by REBUS-PC. Only the accuracy of the flux solution is can be checked given a fully converged system with and without upscattering iterations. Of course, the use of the upscattering iteration should have a notable impact on computational performance.

Much like the A.STP027 input, the output tables also do not need to be verified. As an example, card type 04 simply flags which output tables are to be produced and the fact that the desired output tables are produced by the software, as described later in this section, is sufficient proof that the controls are working. Of all of the A.DIF3D input, only the total power value used by REBUS-PC needs to be verified, which is covered in capabilities 1 and 7. To accomplish this, the analytical test cases are used to verify the reported power and flux magnitude are consistent with the expected values given the provided input data: capture & fission rate power conversion factors. In conclusion, the only important aspect of this input data set to verify is that the selected power level is accurately computed by the software.

3.1.3 A.HMG4C Input of REBUS-PC

This section of input controls the cross section homogenization scheme. It has its own title card which is selectively printed when the module is entered. The only physics control that is relevant in this section occurs in the seventh input on card type 02. The user can choose to use a file-wide chi obtained from the base core composition or make a chi based upon the combination of isotopic chi. The limitation of using a file-wide chi is that it does not change with respect to depletion, and if the fuel burnup is high, the energy distribution of fission neutrons can change as U-235 fission is replaced with Pu-239 fission. The example input for MURR is given as

```
UNFORM=A.HMG4C
01   Detail 2008 MURR 12MW NEQ HEU.UALx.24PL,1.52gU/cc, 93.14 wt% U235
02 30000000 1 0 0 0
```

In this example, the user has selected to use the file-chi option which is typical when the fuel burnup is low. As part of the testing, both options must be verified, which is covered by capabilities 2 and 3.

3.1.4 A.NIP3 Input of REBUS-PC

The A.NIP3 input is typically the longest section of input provided to REBUS-PC as it defines both the geometry, compositions, and composition to geometry mapping information. The following excerpt from the MURR input shows at least one of each card type used.

```
01   2008 MURR 10MW HEU.UALx.24PL, 1.52gU/cc, 93.14 wt% U235
02           0      0 700      0 500      0      0      0      0
03           66
04           6      6      3      4      4      4
06  WATER           0.00      6.2832      0      55      0.0000      84.0000
07  CLADI P1001
09      X      1      0.0440
10      CNTRL1CNTRL2
11  CNTRL1      1.00000      0.2891      7      7
13      MEATI U35f 0      7.7512-3U38f 0      3.0819-2MOYf 0      1.0685-2
14      MIX01 MEATI 0.20277      AL-I      0.79723
15  ALUMJ CLADJ
```

In the full input there are typically thousands of type 13 and type 14 cards and hundreds of card types 06 and 15. The first input card is again a title, which is only printed in the geometry processing section of input, and is taken care of at the beginning of the REBUS-PC execution. The card type 02 is used for debug printing, memory container sizes for the input processing, and some additional selection of output edits. Card type 03 selects the geometry type (θ-R-Z in this case) while type 04 selects the boundary conditions applied to that geometry. As discussed previously, capabilities 4 and 5 require that the inputs provided on the type 04 input translate to the correct application and solution in REBUS-PC.

Card type 06 specifies the geometry itself, which assigns regions (WATER in this example) to a given spatial position. Card type 07 allows the user to collect the region-wise information into “areas” for reactor core summary information. Card type 09 specifies the meshing to use on the geometry provided in card type 06. All of these inputs are checked as part of capabilities 1 and 7.

Card types 10 and 11 are for the internal domain boundary conditions and will have to be checked as part of capability 6. These boundary conditions are typically used to properly handle thermal energy

black absorbers (B-10), which the finite difference methodology has difficulty modeling without considerable spatial meshing.

Card types 13 and 14 are used to define compositions and will have to be checked as part of capabilities 1 and 2. Card type 15 is the mapping between compositions and spatial regions and will be checked as part of capabilities 1 and 2. As stated, these input cards form the bulk of the burden of user input. One aspect of the REBUS-PC software is to produce depleted compositions that the user can feed back into other neutronics models, which is what capability 13 refers to. In this regard, the accuracy of that output with regard to using it as input must be verified.

From the combined discussion on A.NIP3 input, it should be clear that most of the capabilities are specifically focused on the accuracy of this input information. In this regard, most of the verification tests completed in this report are focused on problems that have no depletion. Rather, they are simple checks of the underlying solver of the neutron diffusion equation.

3.1.5 A.BURN Input of REBUS-PC

The A.BURN input is the main control section for the fuel cycle and depletion cases. It has specific inputs for equilibrium and non-equilibrium modes of fuel cycle operation and numerous inputs for external cycle operations such as fuel recycle, fabrication, and reprocessing. With respect to the MURR work and the verification requirements, only a subset of those inputs needs to be verified. The following is an excerpt from an example MURR input.

01	10MW University of Missouri Research Reactor (MURR)									
02	0	48000	0	0.001	0.001	0.001	0	3		
03	0	0.0	0.0	2.0	-1.0	2	0			
09	I135	1	DUMP							
10	I135	I35e0	I35f0	I35k0	I35l0					
24	I135	0		134.907						
25	I135	6	XE135	2.931-05						
26	U35f0	U34f0	U35f0	U36f0	U38f0	NP7f0	PU8f0	PU9f0	PU0f0	PU1f0
28		6.0221367+23								
35	A1A01	A1A01	X4A01	1	2					
36	2.0	0.0	1.0		1	1	2			1.0
39	U34f0	1	10	U35f0	1	10	U36f0	1	10	
40	U34f0	2	1.0-3	8						
41	U35f0	U35f0	1.57184E-03	1.0	U35f1	1.57183E-03	1.0			

Card type 01 is a title card that is printed each time a fuel cycle module is entered and is not verified. Card type 02 defines the memory controls, the convergence and iteration limit settings on the region-wise depletion, and the convergence and iteration limits on the cyclic mode fuel cycle operations. Of these inputs, capability 14 requires that the region-wise depletion inputs are followed and that the depletion calculation itself is accurate. The seven-group depletion problem described in Section 2.6 is relied upon to demonstrate this.

Card type 03 defines the cyclic mode details such as fuel cycle length (days) and burnup convergence setting. Because this is a non-equilibrium problem, the verification is focused on card type 36 which specifies the time step information. In this example excerpt, the burnup convergence is set to -1.0. This basically disables the convergence check on burnup, which is not unusual for non-equilibrium problems. The information provided on card type 03 defines the first time step information in a non-equilibrium problem and thus its input and that of card type 36 will have to be verified.

Card types 09, 10, 24, 25, and 28 are used to define a depletion chain and relate it to the set of isotopes provided in the cross section data. These inputs will have to be verified and is covered by capabilities 3 and 14.

Card types 26, 39, 40, and 41 are all used to define the cross section interpolation with respect to burnup. This input and usage of the physical data will be checked as part of capabilities 11, 12, and 14. In this MURR example, the polynomial approximation is used, although most cases use the cubic spline approach.

Card type 35 specifies the compositional assignments to regions as the reactor fuel cycle progresses along with the time step size and number of depletion steps to apply over each time step. This input is the foundation to the non-equilibrium cycle option and is verified by capabilities 3, 11, 12, 13, and 14.

3.1.6 A.SUMMAR Input of REBUS-PC

The A.SUMMAR is an optional input specification and its most valuable output is to provide whole core integral isotopic reaction rates. In the MURR work, this feature is not used and would only loosely fall under capability 7. The following excerpt is taken from one of the verification tests.

DATASET=A.SUMMAR						
01			0	0	999999	-1 0 0 1
04	1	U35A_0U35C_0				
06	U235	FISS	235.044		U35A_0U35C_0	

The card type 01 input specifies memory and debugging controls and additional output tables. Card types 04 and 06 specify how the isotopes are to be mapped for the isotopic output tables produced by the SUMMAR module. From the list of capabilities, the accuracy of this output is not part of the verification. However, given that it produces supplemental input to capability 7, it is included for completeness.

3.1.7 A.ISO and ISOTXS Input of REBUS-PC

The primary means of providing cross section data to REBUS-PC is to use a binary interface file called ISOTXS. The alternative is to include a section of ascii input called A.ISO. This ascii input will simply produce an ISOTXS in the early geometry and input processing from which the code operates as if the user provided that binary ISOTXS file. The verification aspect is only to ensure that both input options work consistently on a given problem, and that the correct answer is produced which falls under capabilities 2 and 3.

3.2 Verification Test #1

The most logical way to discuss the verification process is to describe the input and output for each of the 22 verification tests and explain how it satisfies the verification of each capability. Verification test #1 is a one-group, 1-D core geometry, and was identified previously in this report as 1GCYL_hom. An input excerpt is provided in Figure 3-1. As discussed, the external boundary conditions are specified on the type 04 cards and the internal boundary conditions are specified on the types 10 and 11 cards of the A.NIP3 dataset. The boundary conditions used by REBUS-PC are printed in the model descriptions of the REBUS-PC output as shown in Figure 3-2. As can be seen, REBUS-PC reports that a reflected condition is set for the first boundary condition on the first dimension and an extrapolated one is set for the second boundary condition on the first dimension. In addition, it provides the

extrapolation parameter of 0.4692 as selected by the user input. (This extrapolation value is the default value used from diffusion theory, as indicated in the manual).

To check the spatial region configurations, the region map was printed in the standard output by turning on the third and fourth input flags of the type 04 card in dataset A.DIF3D. The region and zone map is shown in Figure 3-3. The numbers in the first and last row of each table denote the mesh index in the radial direction, while the numbers in between denote the region (or zone) number assigned to each position. In this example, there is a single composition, and thus there is only one region and one zone and one mesh index in the R-direction (i.e. the radial direction). Star symbols (*) mark the region boundaries. Examination of the plotted region map confirms that the positions of individual regions conform to the user specification given in Figure 3-1. The mesh intervals and region volumes were also checked by comparing the values given in the output to those calculated by a hand calculation.

```

UNFORM=A.DIF3D
01 ***** 1GCVL Model
02 10000 11000000
03 0 0 0 0 50
04 1 1 1 00 010 10 110 0 0 0 0
05 1.0E-07 1.0E-07 1.0E-07
06 1.0 1.0E-05 1.0E-05 10.0E+6
DATASET=A.HMG4C
01 TURN OFF HMG4C EDITS
02 60000 0 1 0 0 0
DATASET=A.NIP3
01 ***** 1GCVL Model
02 0 1 37000 0 750000 10000 0 0 0 0
03 20
04 3 4
05 XU 0.4692
06 HMREG 0.00000E+00 1.00000E+01 20
13 MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 PU9A_0 1.0000E-20
13 MEAT1 LFPA_0 1.0000E-20 DUMP_0 1.0000E-20
13 MODA H01A_0 6.6691E-02 O16A_0 3.3346E-02
14 MIXA MEAT1 3.0857E-01 MODA 6.9143E-01
14 FUEL1 MIXA 1.0
15 FUEL1 HMREG
NOSORT=A.ISO
0V ISOTXS * UNDEFINED * 1

```

Figure 3-1. Truncated Input for Verification Test #1

```

      ---  MODEL DESCRIPTION  ---
2      IGOM      GEOMETRY TYPE, 1-D CYLINDRICAL
1      NZONE     NO. OF ZONES (COMPOSITIONS)
1      NREG      NO. OF REGIONS
1      NZCL      NO. OF ZONE CLASSIFICATIONS
1      NCINTI    NO. OF 1ST DIMENSION COARSE MESH INTERVALS
20     NINTI     NO. OF 1ST DIMENSION FINE MESH INTERVALS
1      IMB1      FIRST BOUNDARY CONDITION, FIRST DIMENSION, REFLECTED
2      IMB2      LAST BOUNDARY CONDITION, FIRST DIMENSION, EXTRAPOLATED
1      NBS       NO. OF BUCKLING SPECIFICATIONS
6      NBCS      NO. OF CONSTANTS FOR EXTERNAL BOUNDARIES
1      NIBCS     NO. OF CONSTANTS FOR INTERNAL BOUNDARIES
0      NZWBB     NO. OF BLACKNESS THEORY ZONES
0      NRASS     0/1, REGION ASSIGNMENTS TO COARSE/FINE MESH
      R- DIRECTION MESH INTERVAL BOUNDARIES

1 0.00000E+00  2 5.00000E-01  3 1.00000E+00  4 1.50000E+00  5 2.00000E+00  6 2.50000E+00  7 3.00000E+00
8 3.50000E+00  9 4.00000E+00 10 4.50000E+00 11 5.00000E+00 12 5.50000E+00 13 6.00000E+00 14 6.50000E+00
15 7.00000E+00 16 7.50000E+00 17 8.00000E+00 18 8.50000E+00 19 9.00000E+00 20 9.50000E+00 21 1.00000E+01
      EXTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
      LAST VALUE SHOWN IS USED FOR REMAINING GROUPS
0      LAST      R BOUNDARY
      1 4.69200E-01

```

Figure 3-2. REBUS-PC Verification Test #1 Output Excerpt #1

0	REACTOR REGION BY MESH POINT										MAP FOR PLANES 1 - 1										
0	-DIM																				
R	-DIM																				
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	

1	*	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	*	1

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
0	REACTOR ZONE BY MESH POINT										MAP FOR PLANES 1 - 1										
0	-DIM																				
R	-DIM																				
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	

1	*	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	*	1

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
...																					
0	OUTER	REL. POINT		REL. SUM		EIGENVALUE		POLY.		DOM. RATIO		DOM. RATIO									
	IT. NO.	ERROR		ERROR		CHANGE		ORDER		USED		ESTIMATED		K-EFFECTIVE							
0	1	4.720265E-01		3.019974E-01		2.280016E-01		0		0.000000E+00		0.000000E+00		1.22800157E+00							
0	2	1.615893E-01		8.252843E-02		-4.476960E-02		0		0.000000E+00		3.050590E-01		1.18323197E+00							
...																					
0	18	4.860591E-08		2.628328E-08		-3.067054E-08		0		0.000000E+00		3.919687E-01		1.13174412E+00							
0	OUTER ITERATIONS COMPLETED AT ITERATION 18, ITERATIONS HAVE CONVERGED																				
0	K-EFFECTIVE = 1.13174412115																				
...																					
0	GROUP SUM OF		REAL FLUX FOR		K-EFF PROBLEM FOR PLANE		1 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)														
0	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
0	1	4.92729E+16	4.90017E+16	4.84614E+16	4.76566E+16	4.65939E+16	4.52821E+16	4.37319E+16	4.19560E+16	3.99691E+16											
	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	
	10	11	12	13	14	15	16	17	18												
0	1	3.77874E+16	3.54286E+16	3.29119E+16	3.02577E+16	2.74873E+16	2.46230E+16	2.16876E+16	1.87043E+16	1.56966E+16											
	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	R-AXIS	
	19	20																			

Figure 3-3. REBUS-PC Verification Test #1 Output Excerpt #2

The analytical flux solution $\phi(r)$ of the neutron diffusion equation in a 1-D cylindrical geometry is a Bessel function of the first kind [8]:

$$\phi(r) = CJ_0(B \cdot r), \quad 0 \leq r \leq R. \quad (1)$$

The normalization factor C is defined by the total power input of 10 MW in Figure 3-1. The constant B is defined by the boundary condition at the maximum radius R . The general boundary condition can be expressed as

$$\alpha \vec{n} \cdot \vec{J} \Big|_{\partial V} + \beta \phi \Big|_{\partial V} = \alpha D \phi'(R) + \beta \phi(R) = 0. \quad (2)$$

In this example, an extrapolated boundary condition was used, which REBUS-PC allows a user-specified constant $A = \beta / \alpha$. The zero flux boundary condition ($\alpha = 0$ and $\beta = 1$) requires a specific boundary condition input, where as this input path allows any result between zero flux condition and the reflected condition ($\alpha = 1$ and $\beta = 0$). As discussed previously, the default extrapolation factor $A = 0.4692$ was used, as evident from the output file.

Inserting equation 1 into equation 2 produces

$$-\alpha DBJ_1(BR) + \beta J_0(BR) = 0, \quad (3)$$

where $J_1(BR)$ is the first-order Bessel function of the first kind. With a given constant A , equation 3 can be solved for the first positive root of B using the Wolfram Mathematica program [9] or MathCAD [10]. With the obtained geometric buckling, B^2 , the analytical k-effective can be defined as

$$k_{eff} = \nu \Sigma_f / (\Sigma_r + DB^2). \quad (4)$$

The finite difference methodology is not an analytic methodology and thus the solutions are dependent upon the mesh refinement. As such, equally spaced mesh refinement is used which should provide asymptotic convergence as opposed to gradient based meshing. In this regard, the input must be modified and executed several times to verify accuracy with respect to the analytic solution. Table 3-1 presents the results of this mesh refinement work for a zero flux boundary condition and two different extrapolation boundary conditions. As discussed in the preceding theory section, the analytic result was obtained using Mathematica and MathCAD.

Table 3-1. Analytic and Computed Eigenvalue Results for Verification Test #1

Boundary Condition			Zero Flux at R	Extrapolated Condition at R	
			$\alpha=0, \beta=1$	$A=\beta/\alpha=0.5$	$A=\beta/\alpha=0.4692$
REBUS-PC	Mesh Size (cm)	1.00	1.0203692	1.1262925	1.1326695
		0.50	1.0193621	1.1253599	1.1317441
		0.25	1.0191104	1.1251268	1.1315128
	Richardson Extrapolation		1.0190266	1.1250491	1.1314358
Analytic Solution			1.0190266	1.1250491	1.1314358

Because this is a simple bare core geometry, it is more sensitive to mesh refinement than typical reactor problems, and thus this is an excellent choice for demonstrating the accuracy limitations of the finite difference methodology. As can be seen, the coarser the meshing in REBUS-PC, the larger the error with respect to the analytic solution. A Richardson Extrapolation [11] result based upon the

three mesh results obtained with REBUS-PC is provided to demonstrate that with a zero mesh size, the REBUS-PC methodology will result in the correct solution.

The verification test corresponds to a mesh size of 0.5 cm and $A=0.4692$. From the output excerpt in Figure 3-3 one finds the eigenvalue matches that provided in Table 3-1. In addition to this basic check, the average flux results reported by REBUS-PC are also compared. Figure 3-3 shows the mesh averaged flux output edit from REBUS-PC which is compared against the analytic result taken from the MathCAD worksheet provided in the repository with the first verification test. Table 3-2 shows the comparison of the flux result and resulting error. As can be seen, the error is largest near the extrapolated boundary condition peaking at 0.034% error and, because of the normalization constraint, it becomes negative as it approaches the core center. This type of result is not surprising given the mesh size chosen and the gradient in the flux.

Table 3-2. Mesh Averaged Flux Comparisons For Verification Test #1

Mesh No.	REBUS-PC Results	Analytical Results	Error
1	4.92729E+16	4.92679E+16	-0.010%
2	4.90017E+16	4.89967E+16	-0.010%
3	4.84614E+16	4.84566E+16	-0.010%
4	4.76566E+16	4.76520E+16	-0.010%
5	4.65939E+16	4.65896E+16	-0.009%
6	4.52821E+16	4.52781E+16	-0.009%
7	4.37319E+16	4.37282E+16	-0.008%
8	4.19560E+16	4.19528E+16	-0.008%
9	3.99691E+16	3.99664E+16	-0.007%
10	3.77874E+16	3.77851E+16	-0.006%
11	3.54286E+16	3.54269E+16	-0.005%
12	3.29119E+16	3.29107E+16	-0.004%
13	3.02577E+16	3.02571E+16	-0.002%
14	2.74873E+16	2.74873E+16	0.000%
15	2.46230E+16	2.46236E+16	0.002%
16	2.16876E+16	2.16887E+16	0.005%
17	1.87043E+16	1.87060E+16	0.009%
18	1.56966E+16	1.56989E+16	0.015%
19	1.26881E+16	1.26908E+16	0.022%
20	9.70181E+15	9.70508E+15	0.034%

For completeness, the comparison results for a finer mesh solution for $A=0.5$ in provided in Table 3-3. This calculation is not part of the repository. Relative to the results for the coarser mesh in Table 3-2, the agreement between REBUS-PC and the analytic solution in Table 3-3 are almost an order of magnitude better, with a maximum error of 0.011% at the core edge. Combined, these results demonstrate that the flux solution methodology in REBUS-PC is accurate and correctly implemented with regard to the cross sections and power normalization constraint provided by the user. Because this verification test uses the 1-D cylindrical geometry in REBUS-PC, it does not satisfy any stated capability, although the exact same test can be used with the correct 3-D geometry in REBUS-PC with proper boundary conditions.

Table 3-3. Mesh Averaged Flux Comparisons For Altered Verification Test #1

Mesh No.	REBUS-PC Results	Analytical Results	Error
1	4.98723E+16	4.98709E+16	-0.0028%
2	4.98025E+16	4.98011E+16	-0.0028%
3	4.96631E+16	4.96617E+16	-0.0028%
4	4.94543E+16	4.94530E+16	-0.0026%
5	4.91767E+16	4.91753E+16	-0.0028%
6	4.88307E+16	4.88294E+16	-0.0027%
7	4.84172E+16	4.84158E+16	-0.0029%
8	4.79369E+16	4.79356E+16	-0.0027%
9	4.73909E+16	4.73896E+16	-0.0027%
10	4.67803E+16	4.67791E+16	-0.0026%
11	4.61064E+16	4.61052E+16	-0.0026%
12	4.53706E+16	4.53695E+16	-0.0024%
13	4.45745E+16	4.45734E+16	-0.0025%
14	4.37196E+16	4.37186E+16	-0.0023%
15	4.28079E+16	4.28070E+16	-0.0021%
16	4.18411E+16	4.18403E+16	-0.0019%
17	4.08214E+16	4.08206E+16	-0.0020%
18	3.97507E+16	3.97500E+16	-0.0018%
19	3.86314E+16	3.86308E+16	-0.0016%
20	3.74658E+16	3.74652E+16	-0.0016%
21	3.62562E+16	3.62557E+16	-0.0014%
22	3.50052E+16	3.50047E+16	-0.0014%
23	3.37153E+16	3.37149E+16	-0.0012%
24	3.23892E+16	3.23889E+16	-0.0009%
25	3.10296E+16	3.10294E+16	-0.0006%
26	2.96393E+16	2.96392E+16	-0.0003%
27	2.82211E+16	2.82211E+16	0.0000%
28	2.67779E+16	2.67780E+16	0.0004%
29	2.53127E+16	2.53129E+16	0.0008%
30	2.38284E+16	2.38286E+16	0.0008%
31	2.23281E+16	2.23283E+16	0.0009%
32	2.08146E+16	2.08150E+16	0.0019%
33	1.92911E+16	1.92915E+16	0.0021%
34	1.77606E+16	1.77611E+16	0.0028%
35	1.62261E+16	1.62267E+16	0.0037%
36	1.46908E+16	1.46915E+16	0.0048%
37	1.31575E+16	1.31583E+16	0.0061%
38	1.16294E+16	1.16302E+16	0.0069%
39	1.01094E+16	1.01102E+16	0.0079%
40	8.60037E+15	8.60131E+15	0.0109%

3.3 Verification Test #2

Verification test #2 is also a one-group, 1-D geometry, but it uses the internal black absorber boundary condition. This problem was previously identified as 1GCYL_black. The external boundary conditions are specified on the type 04 cards and the internal boundary conditions are specified on the types 10 and 11 cards of A.NIP3, as seen in Figure 3-4. The boundary conditions used by REBUS-PC are printed in the model descriptions of the REBUS-PC output, and are shown in Figure 3-5. As can be seen, REBUS-PC reports that a reflected condition is set for the first boundary condition on the first dimension and an extrapolated one is set for the second boundary condition on the first dimension with an extrapolation parameter of 0.4692 (the default). The black boundary condition setup is also reported in Figure 3-5, indicating the user input of Figure 3-4 is accepted and used by the software.

```

UNFORM=A.DIF3D
01 ***** 1GCYL Model *****
02 10000 11000000
03 0 0 0 0 50
04 1 1 1 00 010 10 110 0 0 0 0
05 1.0E-07 1.0E-07 1.0E-07
06 1.0 1.0E-05 1.0E-05 10.0E+6
DATASET=A.HMG4C
01 TURN OFF HMG4C EDITS
02 60000 0 1 0 0 0
DATASET=A.NIP3
01 ***** 1GCYL Model *****
02 0 1 37000 0 750000 10000 0 0 0 0
03 20
04 3 4
06 REGN1 0.00000E+00 1.00000E+01 20
06 REGN2 1.00000E+01 1.10000E+01 2
10 BLACK
11 BLACK 1.0 0.4692
13 MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 PU9A_0 1.0000E-20
13 MEAT1 LFPA_0 1.0000E-20 DUMP_0 1.0000E-20
13 MODA H01A_0 6.6691E-02 O16A_0 3.3346E-02
14 MIXA MEAT1 3.0857E-01 MODA 6.9143E-01
14 FUEL1 MIXA 1.0
14 BLACK MODA 1.0
15 FUEL1 REGN1
15 BLACK REGN2
...

```

Figure 3-4. Truncated Input for Verification Test #2

In DIF3D, the internal black absorber condition is specified similar to the external boundary condition:

$$\alpha \vec{n} \cdot \vec{J}|_s + \beta \phi|_s = 0, \quad (5)$$

where $\vec{J}|_s$ and $\phi|_s$ are the current and flux on the internal boundary. By introducing an extrapolated boundary condition with the same constant $A = \beta / \alpha$ on the interface, the same analytic solution obtained in 1GCYL_hom will be obtained.

```

      ---  MODEL DESCRIPTION  ---
      2      IGOM      GEOMETRY TYPE, 1-D CYLINDRICAL
      2      NZONE     NO. OF ZONES (COMPOSITIONS)
      2      NREG      NO. OF REGIONS
      1      NZCL      NO. OF ZONE CLASSIFICATIONS
      2      NCINTI     NO. OF 1ST DIMENSION COARSE MESH INTERVALS
      22     NINTI     NO. OF 1ST DIMENSION FINE MESH INTERVALS
      1      IMB1      FIRST BOUNDARY CONDITION, FIRST DIMENSION, REFLECTED
      2      IMB2      LAST BOUNDARY CONDITION, FIRST DIMENSION, EXTRAPOLATED
      1      NBS       NO. OF BUCKLING SPECIFICATIONS
      1      NBCS      NO. OF CONSTANTS FOR EXTERNAL BOUNDARIES
      1      NIBCS     NO. OF CONSTANTS FOR INTERNAL BOUNDARIES
      1      NZWBB     NO. OF BLACKNESS THEORY ZONES
      0      NRASS     0/1, REGION ASSIGNMENTS TO COARSE/FINE MESH

      R- DIRECTION MESH INTERVAL BOUNDARIES
      1 0.00000E+00  2 5.00000E-01  3 1.00000E+00  4 1.50000E+00  5 2.00000E+00  6 2.50000E+00  7 3.00000E+00
      8 3.50000E+00  9 4.00000E+00 10 4.50000E+00 11 5.00000E+00 12 5.50000E+00 13 6.00000E+00 14 6.50000E+00
      15 7.00000E+00 16 7.50000E+00 17 8.00000E+00 18 8.50000E+00 19 9.00000E+00 20 9.50000E+00 21 1.00000E+01
      22 1.05000E+01 23 1.10000E+01

      EXTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
      LAST VALUE SHOWN IS USED FOR REMAINING GROUPS
      LAST      R BOUNDARY
      1 4.69200E-01

      REGION/ZONE SPECIFICATIONS
      REGION REGION REGION ZONE ZONE ZONE
      NO. NAME VOLUME NO. NAME CLASS. BUCKLING BY GROUP
      1 REGN1 3.142E+02 1 FUEL1 0 0.000E+00
      2 REGN2 6.597E+01 2 BLACK 0 0.000E+00

      INTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
      LAST VALUE SHOWN IS USED FOR REMAINING GROUPS
      1 4.69200E-01

      BLACKNESS THEORY ZONE NUMBERS AND LABELS
      ZONE ZONE ZONE ZONE ZONE ZONE
      NO. NAME NO. NAME NO. NAME NO. NAME NO. NAME NO. NAME
      2 BLACK

      ...
      0      OUTER ITERATIONS COMPLETED AT ITERATION 18, ITERATIONS HAVE CONVERGED
      0      K-EFFECTIVE = 1.13174412115
      0      GROUP SUM OF REAL FLUX FOR K-EFF PROBLEM FOR PLANE 1 WITH ENERGY RANGE (EV)
      0      R-AXIS R-AXIS R-AXIS R-AXIS R-AXIS R-AXIS R-AXIS ...
      1      2 3 4 5 6 ...

      1 4.92729E+16 4.90017E+16 4.84614E+16 4.76566E+16 4.65939E+16 4.52821E+16 ...

```

Figure 3-5. REBUS-PC Verification Test #2 Output Excerpt

Table 3-4 shows the k-effective results of the 1GCYL_hom and 1GCYL_black problems for two different extrapolated boundary condition settings. The eigenvalue result shown is also provided in the output excerpt of Figure 3-5. The consistent k-effective results confirm that the internal black absorber condition is implemented correctly in REBUS-PC. Because this verification test again uses the 1-D cylinder geometry in REBUS-PC, it does not satisfy any stated capability, although it can be converted to the desired 3-D geometry in REBUS-PC with proper boundary conditions.

Table 3-4. Comparison of k-effective Values of 1GCYL_hom and 1GCYL_black Models

Problem	A=0.5	A=0.4692
1GCYL_hom	1.1253599	1.1317441
1GCYL_black	1.1253599	1.1317441

3.4 Verification Test #3

Verification test #3 is the 3-D θ -R-Z geometry representation of test #1. To accomplish this, reflected boundary conditions are introduced in the Z direction and periodic boundary conditions are used in the θ direction. Figure 3-6 shows the truncated input for verification test #3. Comparing Figure 3-1 to Figure 3-6 one finds the only real differences are in card types 03 through 06 and 09 of the A.NIP3 input.

```

UNFORM=A.DIF3D
01 ***** 1GCRYL Model *****
02      10000 11000000
03      0      0      0      0      50
04      1      1      1      00      010      10      110      0      0      0      0
05      1.0E-07      1.0E-07      1.0E-07
06      1.0      1.0E-05      1.0E-05      10.0E+6
DATASET=A.HMG4C
01      TURN OFF HMG4C EDITS
02      60000      0      1      0      0      0
DATASET=A.NIP3
01 ***** 1GCRYL to TRZ Model *****
02      0      1 37000      0 750000 10000      0      0      0      0
03      66
04      6      6      3      4      3      3
05      YU 0.4692
06      HMREG 0.00000E+00 6.283185310      0      4      0.00000E+00 1.00000E+01
09      X      12 6.283185310
09      Y      20 1.00000E+01
09      Z      4 1.000000000
13      MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 PU9A_0 1.0000E-20
13      MEAT1 LFPA_0 1.0000E-20 DUMP_0 1.0000E-20
13      MODA H01A_0 6.6691E-02 O16A_0 3.3346E-02
14      MIXA MEAT1 3.0857E-01 MODA 6.9143E-01
14      FUEL1 MIXA 1.0
14      BLACK MODA 1.0
15      FUEL1 REGN1
15      BLACK REGN2
...

```

Figure 3-6. Truncated Input for Verification Test #3

On card type 03, geometry type 66 is chosen (3-D) instead of 20 (1-D cylinder). On card type 04, because it is a 3-D geometry, there are more boundary conditions, where R is ordered second in θ -R-Z. This means that the earlier boundary conditions now appear as the third and fourth inputs on the same line. For θ , a type 6 boundary condition is used while for Z a type 3 is used. Type 3 is reflected while type 6 is periodic repeating with the opposite face. For type 6, the opposite surface means the lower or upper surface of the given dimension (+X with -X as an example) noting that type 7 is periodic adjacent and is intended to connect directions X and Y. Because of the change in order of the R dimension, the card type 05 input is altered to point the extrapolated boundary condition to the upper Y dimension (actually R) instead of the upper X dimension.

The card type 06 and 09 changes are associated with the way DIF3D accepts 3-D input. Instead of providing the consecutive coordinates for a given region, card type 06 requires the X and Y coordinates in centimeters and the Z plane locations. In this regard, the "0 4" at the middle of the card type 06 specifies the region occupies planes 1-4 between Z surfaces 0 and 4. The actual coordinates of those surfaces are specified on card type 09. Because a reflected boundary condition was chosen

for all surfaces in Z, the actual dimension is not important. A value of 1.0 was chosen for simplicity. For θ , the entire domain (2π) is specified to keep the same power scaling as verification test #1.

The output from verification test #3 is much larger than that of #1 because there are $12 \times 20 \times 4$ meshes instead of 20 meshes. The model description excerpt is provided in Figure 3-7 and sections of the flux and power tables in Figure 3-8. Starting with the model description, one can see that the input provided is correctly reported as θ -R-Z; the geometry type number changes to 15 from 66, as 15 is the standard ID of this geometry type in GEODST. The number of meshes, $12 \times 20 \times 4$ is reiterated, as is the boundary condition information, the numbers of which again change from the input values due to the GEODST standard ID. It is important to note that REBUS-PC reports the boundary conditions using the naming (REFLECTIVE, PERIODIC, etc...) rather than just the numerical ID. The mesh intervals REBUS-PC uses are also reported correctly and consistently with the input, as is the region volume: $\pi(10\text{ cm})^2 \cdot 1\text{ cm} = 314.15926536$. The last part of output provided in Figure 3-7 is the eigenvalue convergence section which shows a final eigenvalue (1.13174412115) identical to the eigenvalue from verification test #1 (1.13174412115), and consistent with the analytic solution (1.1314358). The previous zero mesh extrapolation applied here yields the same results as that observed in verification test #1.

As can be inferred from the identical eigenvalue and problem setup, the flux solution is also identical as observed in Figure 3-8 and the tabulated data from verification tests #1 and #3 in Table 3-5. This result is not the expected outcome, as REBUS-PC uses an iterative solution technique and there can be some variance in the final converged result. Given the consistent results, along with the extended testing, this test demonstrates that REBUS-PC is correctly solving the θ -R-Z geometry.

It is important to note in Figure 3-8 that the flux solution at all θ and Z values are identical. This is a result of the reflected and periodic boundary conditions being applied in both directions, leading to a flat flux approximation. In this regard, this analytic benchmark problem is not a full test of the implementation of a θ -R-Z finite difference solution algorithm. Because analytic solutions with a fission source are hard to create, fixed source cases are used to fulfill that need, and are shown later.

In addition to the average flux by mesh, the total flux and peak flux values reported by REBUS-PC are compared against the analytic benchmark. The peak occurs at the center of the domain and is calculated to be $4.989\text{E}+16$, where REBUS-PC returns $4.927\text{E}+16$, or a 1.2% error. Using a finer mesh, as done in verification test #1, yields $4.932\text{E}+16$, which is somewhat closer to the analytic result. Using 120 meshes yields $4.933\text{E}+16$, indicating that REBUS-PC will never quite reach the analytic solution result. The total flux reported by REBUS-PC is $8.39223\text{E}+18$ for all three inputs while the analytic result is also $8.39223\text{E}+18$. This is consistent with the normalization constraint.

To understand the peak flux error issue, one must understand that DIF3D does not evaluate the flux at the center of the mesh, but uses the current at the mesh edges and mesh averaged flux (mesh center) to estimate the peak flux. In this regard the peak flux estimate is only somewhat reliable, although still rather accurate for this test. Of all the methodologies in DIF3D, DIF3D-VARIANT is the only one that can allow a rigorous evaluation of the peak flux. The implemented technique, chosen for speed, is an approximation and thus produces a result with similar errors seen above. Given that the peaking calculation is denoted in both the output and the manual as an approximation, the preceding check is considered sufficient verification that the outputs produced by the REBUS-PC software are correct.

```

15      IGOM      GEOMETRY TYPE, THETA-R-Z
1      NZONE      NO. OF ZONES (COMPOSITIONS)
1      NREG       NO. OF REGIONS
1      NZCL       NO. OF ZONE CLASSIFICATIONS
1      NCINTI     NO. OF 1ST DIMENSION COARSE MESH INTERVALS
1      NCINTJ     NO. OF 2ND DIMENSION COARSE MESH INTERVALS
1      NCINTK     NO. OF 3RD DIMENSION COARSE MESH INTERVALS
12     NINTI      NO. OF 1ST DIMENSION FINE MESH INTERVALS
20     NINTJ      NO. OF 2ND DIMENSION FINE MESH INTERVALS
4      NINTK      NO. OF 3RD DIMENSION FINE MESH INTERVALS
3      IMB1       FIRST BOUNDARY CONDITION, FIRST DIMENSION, PERIODIC, OPPOSITE FACE
3      IMB2       LAST BOUNDARY CONDITION, FIRST DIMENSION, PERIODIC, OPPOSITE FACE
1      JMB1       FIRST BOUNDARY CONDITION, SECOND DIMENSION, REFLECTED
2      JMB2       LAST BOUNDARY CONDITION, SECOND DIMENSION, EXTRAPOLATED
1      KMB1       FIRST BOUNDARY CONDITION, THIRD DIMENSION, REFLECTED
1      KMB2       LAST BOUNDARY CONDITION, THIRD DIMENSION, REFLECTED
1      NBS        NO. OF BUCKLING SPECIFICATIONS
6      NBCS       NO. OF CONSTANTS FOR EXTERNAL BOUNDARIES
1      NIBCS      NO. OF CONSTANTS FOR INTERNAL BOUNDARIES
0      NZWBB      NO. OF BLACKNESS THEORY ZONES
0      NRASS      0/1, REGION ASSIGNMENTS TO COARSE/FINE MESH

              THETA- DIRECTION MESH INTERVAL BOUNDARIES
1 0.00000E+00  2 5.23599E-01  3 1.04720E+00  4 1.57080E+00  5 2.09440E+00  6 2.61799E+00  7 3.14159E+00
8 3.66519E+00  9 4.18879E+00 10 4.71239E+00 11 5.23599E+00 12 5.75959E+00 13 6.28319E+00

              R- DIRECTION MESH INTERVAL BOUNDARIES
1 0.00000E+00  2 5.00000E-01  3 1.00000E+00  4 1.50000E+00  5 2.00000E+00  6 2.50000E+00  7 3.00000E+00
8 3.50000E+00  9 4.00000E+00 10 4.50000E+00 11 5.00000E+00 12 5.50000E+00 13 6.00000E+00 14 6.50000E+00
15 7.00000E+00 16 7.50000E+00 17 8.00000E+00 18 8.50000E+00 19 9.00000E+00 20 9.50000E+00 21 1.00000E+01

              Z- DIRECTION MESH INTERVAL BOUNDARIES
1 0.00000E+00  2 2.50000E-01  3 5.00000E-01  4 7.50000E-01  5 1.00000E+00
...

              REGION/ZONE SPECIFICATIONS
              REGION  REGION  REGION  ZONE  ZONE  ZONE
              NO.    NAME  VOLUME  NO.   NAME  CLASS.
              1      HMREG  3.142E+02  1    FUEL1  0
              BUCKLING BY GROUP (REPEAT LAST VALUE FOR REMAINING GROUPS)
              0.000E+00

...
0      OUTER      REL. POINT      REL. SUM      EIGENVALUE      POLY.      DOM. RATIO      DOM. RATIO
IT. NO.      ERROR      ERROR      CHANGE      ORDER      USED      ESTIMATED      K-EFFECTIVE
0      1      4.720260E-01  3.019970E-01  2.280010E-01  0      0.000000E+00  0.000000E+00  1.22800103E+00
...
0      18      4.860733E-08  2.628403E-08  -3.067128E-08  0      0.000000E+00  3.919694E-01  1.13174412E+00
0      OUTER ITERATIONS COMPLETED AT ITERATION 18, ITERATIONS HAVE CONVERGED
0      K-EFFECTIVE = 1.13174412115

```

Figure 3-7. REBUS-PC Verification Test #3 Output Excerpt #1

REGION NO.	NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC) (2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION					
1	HMREG	1	HMREG	3.14159E+02	1.00000E+00	1.00000E+07	3.18310E+04	5.87125E+04	1.84451E+00	1.00000E+00					
TOTALS				3.14159E+02	0.00000E+00	1.00000E+07	3.18310E+04	5.87125E+04	1.84451E+00	1.00000E+00					
...															
0	GROUP SUM OF REAL FLUX FOR K-EFF PROBLEM FOR PLANE 1 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)														
0	R-AXIS	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA					
		1	2	3	4	5	6	7	8	9					
20		9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15					
19		1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16					
18		1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16					
17		1.87043E+16	1.87043E+16	1.87043E+16	1.87043E+16	1.87043E+16	1.87043E+16	1.87043E+16	1.87043E+16	1.87043E+16					
16		2.16876E+16	2.16876E+16	2.16876E+16	2.16876E+16	2.16876E+16	2.16876E+16	2.16876E+16	2.16876E+16	2.16876E+16					
15		2.46230E+16	2.46230E+16	2.46230E+16	2.46230E+16	2.46230E+16	2.46230E+16	2.46230E+16	2.46230E+16	2.46230E+16					
14		2.74873E+16	2.74873E+16	2.74873E+16	2.74873E+16	2.74873E+16	2.74873E+16	2.74873E+16	2.74873E+16	2.74873E+16					
13		3.02577E+16	3.02577E+16	3.02577E+16	3.02577E+16	3.02577E+16	3.02577E+16	3.02577E+16	3.02577E+16	3.02577E+16					
12		3.29119E+16	3.29119E+16	3.29119E+16	3.29119E+16	3.29119E+16	3.29119E+16	3.29119E+16	3.29119E+16	3.29119E+16					
11		3.54286E+16	3.54286E+16	3.54286E+16	3.54286E+16	3.54286E+16	3.54286E+16	3.54286E+16	3.54286E+16	3.54286E+16					
10		3.77874E+16	3.77874E+16	3.77874E+16	3.77874E+16	3.77874E+16	3.77874E+16	3.77874E+16	3.77874E+16	3.77874E+16					
9		3.99691E+16	3.99691E+16	3.99691E+16	3.99691E+16	3.99691E+16	3.99691E+16	3.99691E+16	3.99691E+16	3.99691E+16					
8		4.19560E+16	4.19560E+16	4.19560E+16	4.19560E+16	4.19560E+16	4.19560E+16	4.19560E+16	4.19560E+16	4.19560E+16					
7		4.37319E+16	4.37319E+16	4.37319E+16	4.37319E+16	4.37319E+16	4.37319E+16	4.37319E+16	4.37319E+16	4.37319E+16					
6		4.52821E+16	4.52821E+16	4.52821E+16	4.52821E+16	4.52821E+16	4.52821E+16	4.52821E+16	4.52821E+16	4.52821E+16					
5		4.65939E+16	4.65939E+16	4.65939E+16	4.65939E+16	4.65939E+16	4.65939E+16	4.65939E+16	4.65939E+16	4.65939E+16					
4		4.76566E+16	4.76566E+16	4.76566E+16	4.76566E+16	4.76566E+16	4.76566E+16	4.76566E+16	4.76566E+16	4.76566E+16					
3		4.84614E+16	4.84614E+16	4.84614E+16	4.84614E+16	4.84614E+16	4.84614E+16	4.84614E+16	4.84614E+16	4.84614E+16					
2		4.90017E+16	4.90017E+16	4.90017E+16	4.90017E+16	4.90017E+16	4.90017E+16	4.90017E+16	4.90017E+16	4.90017E+16					
1		4.92729E+16	4.92729E+16	4.92729E+16	4.92729E+16	4.92729E+16	4.92729E+16	4.92729E+16	4.92729E+16	4.92729E+16					
...															
0	GROUP SUM OF REAL FLUX FOR K-EFF PROBLEM FOR PLANE 2 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)														
0	R-AXIS	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA					
		1	2	3	4	5	6	7	8	9					
20		9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15	9.70181E+15					
19		1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16	1.26881E+16					
18		1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16	1.56966E+16					
...															
REGION NO.	NAME	ZONE NO.	ZONE NAME	NET LEAKAGE	+	ABSORPTION RATE(1)	SCATTER OUT(2)	-	SCATTER IN	-	FISSION PRODUCTION(3)	-	EXTERNAL SOURCE	=	BALANCE
1	HMREG	1	HMREG	2.42664E+17		4.44565E+17	-1.46086E+14		0.00000E+00		6.87082E+17		0.00000E+00		1.89629E+10
TOTALS				2.42664E+17		4.44565E+17	-1.46086E+14		0.00000E+00		6.87082E+17		0.00000E+00		1.89629E+10
...															
REGION NO.	NAME	ZONE NO.	ZONE NAME	VOLUME (CC)		TOTAL FLUX (NEUTRON-CM/SEC)	PEAK FLUX (1) (NEUTRON/CM2-SEC)		TOTAL FAST FLUX (NEUTRON-CM/SEC)		PEAK FAST FLUX(1) (NEUTRON/CM2-SEC)				
1	HMREG	1	HMREG	3.14159E+02		8.39223E+18	4.92729E+16		0.00000E+00		0.00000E+00				
TOTALS				3.14159E+02		8.39223E+18	4.92729E+16		0.00000E+00		0.00000E+00				
...															

Figure 3-8. REBUS-PC Verification Test #3 Output Excerpt #2

Table 3-5. Mesh Averaged Flux Comparisons for Verification Test #3

Mesh No.	REBUS-PC Verification Test #1	REBUS-PC Verification Test #3	Analytical Results	Error
1	4.92729E+16	4.92729E+16	4.92679E+16	-0.010%
2	4.90017E+16	4.90017E+16	4.89967E+16	-0.010%
3	4.84614E+16	4.84614E+16	4.84566E+16	-0.010%
4	4.76566E+16	4.76566E+16	4.76520E+16	-0.010%
5	4.65939E+16	4.65939E+16	4.65896E+16	-0.009%
6	4.52821E+16	4.52821E+16	4.52781E+16	-0.009%
7	4.37319E+16	4.37319E+16	4.37282E+16	-0.008%
8	4.19560E+16	4.19560E+16	4.19528E+16	-0.008%
9	3.99691E+16	3.99691E+16	3.99664E+16	-0.007%
10	3.77874E+16	3.77874E+16	3.77851E+16	-0.006%
11	3.54286E+16	3.54286E+16	3.54269E+16	-0.005%
12	3.29119E+16	3.29119E+16	3.29107E+16	-0.004%
13	3.02577E+16	3.02577E+16	3.02571E+16	-0.002%
14	2.74873E+16	2.74873E+16	2.74873E+16	0.000%
15	2.46230E+16	2.46230E+16	2.46236E+16	0.002%
16	2.16876E+16	2.16876E+16	2.16887E+16	0.005%
17	1.87043E+16	1.87043E+16	1.87060E+16	0.009%
18	1.56966E+16	1.56966E+16	1.56989E+16	0.015%
19	1.26881E+16	1.26881E+16	1.26908E+16	0.022%
20	9.70181E+15	9.70181E+15	9.70508E+15	0.034%

With the preceding results, this verification test demonstrates the following capabilities:

- Capability 1, as it compares an analytic eigenvalue based reference solution with the underlying finite difference approximation in REBUS-PC
- Capability 4, as the analytic benchmark requires the reflected boundary condition in R to work correctly in order to get the answer.
- Capability 5 is partially satisfied, as it demonstrates the extrapolated boundary condition in R works in order for it to match the analytic solution
- Capability 7 is partially satisfied, as it demonstrates the output edits for flux are consistent with the analytic solution.

The power calculation in this verification test only considers a simple scaling of the flux for one region and it is not considered a rigorous test of the stated capability 7 as intended.

3.5 Verification Test #4

Verification test #4 is the 3-D θ -R-Z geometry representation of test #2. The same approach used to convert test #1 into #3 is used. Consequently, the excerpt of the input is omitted as it is a simple repeat of previous discussion of test #2. Figure 3-9 provides part of the output from the verification test and one finds the eigenvalue exactly matches the value of 1.1317441 in Table 3-4. Additionally, one can see that the flux solution result exactly matches that provided in Table 3-5 except for the additional 0.0 flux values, which are associated with the black absorber region. The same meshing and appropriate boundary conditions are used to reproduce the results in Table 3-4.

```

0      15      8.071396E-07  4.364468E-07 -5.092886E-07  0  0.000000E+00  3.919762E-01  1.13174443E+00
0      16      3.163731E-07  1.710750E-07 -1.996290E-07  0  0.000000E+00  3.919722E-01  1.13174423E+00
0      17      1.240083E-07  6.705634E-08 -7.824900E-08  0  0.000000E+00  3.919703E-01  1.13174415E+00
0      18      4.860733E-08  2.628403E-08 -3.067128E-08  0  0.000000E+00  3.919694E-01  1.13174412E+00
0      OUTER ITERATIONS COMPLETED AT ITERATION 18, ITERATIONS HAVE CONVERGED
0      K-EFFECTIVE = 1.13174412115
0      REGION/ZONE SPECIFICATIONS
...
0      GROUP SUM OF REAL FLUX FOR K-EFF PROBLEM FOR PLANE 1 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)
0  R-AXIS THETA THETA THETA THETA THETA THETA THETA THETA THETA THETA
      1 2 3 4 5 6 7 8 9
22 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
21 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
20 9.70181E+15 9.70181E+15 9.70181E+15 9.70181E+15 9.70181E+15 9.70181E+15 9.70181E+15 9.70181E+15 9.70181E+15
19 1.26881E+16 1.26881E+16 1.26881E+16 1.26881E+16 1.26881E+16 1.26881E+16 1.26881E+16 1.26881E+16 1.26881E+16
18 1.56966E+16 1.56966E+16 1.56966E+16 1.56966E+16 1.56966E+16 1.56966E+16 1.56966E+16 1.56966E+16 1.56966E+16
17 1.87043E+16 1.87043E+16 1.87043E+16 1.87043E+16 1.87043E+16 1.87043E+16 1.87043E+16 1.87043E+16 1.87043E+16
16 2.16876E+16 2.16876E+16 2.16876E+16 2.16876E+16 2.16876E+16 2.16876E+16 2.16876E+16 2.16876E+16 2.16876E+16
15 2.46230E+16 2.46230E+16 2.46230E+16 2.46230E+16 2.46230E+16 2.46230E+16 2.46230E+16 2.46230E+16 2.46230E+16
14 2.74873E+16 2.74873E+16 2.74873E+16 2.74873E+16 2.74873E+16 2.74873E+16 2.74873E+16 2.74873E+16 2.74873E+16
13 3.02577E+16 3.02577E+16 3.02577E+16 3.02577E+16 3.02577E+16 3.02577E+16 3.02577E+16 3.02577E+16 3.02577E+16
12 3.29119E+16 3.29119E+16 3.29119E+16 3.29119E+16 3.29119E+16 3.29119E+16 3.29119E+16 3.29119E+16 3.29119E+16
11 3.54286E+16 3.54286E+16 3.54286E+16 3.54286E+16 3.54286E+16 3.54286E+16 3.54286E+16 3.54286E+16 3.54286E+16
10 3.77874E+16 3.77874E+16 3.77874E+16 3.77874E+16 3.77874E+16 3.77874E+16 3.77874E+16 3.77874E+16 3.77874E+16
9 3.99691E+16 3.99691E+16 3.99691E+16 3.99691E+16 3.99691E+16 3.99691E+16 3.99691E+16 3.99691E+16 3.99691E+16
8 4.19560E+16 4.19560E+16 4.19560E+16 4.19560E+16 4.19560E+16 4.19560E+16 4.19560E+16 4.19560E+16 4.19560E+16
7 4.37319E+16 4.37319E+16 4.37319E+16 4.37319E+16 4.37319E+16 4.37319E+16 4.37319E+16 4.37319E+16 4.37319E+16
6 4.52821E+16 4.52821E+16 4.52821E+16 4.52821E+16 4.52821E+16 4.52821E+16 4.52821E+16 4.52821E+16 4.52821E+16
5 4.65939E+16 4.65939E+16 4.65939E+16 4.65939E+16 4.65939E+16 4.65939E+16 4.65939E+16 4.65939E+16 4.65939E+16
4 4.76566E+16 4.76566E+16 4.76566E+16 4.76566E+16 4.76566E+16 4.76566E+16 4.76566E+16 4.76566E+16 4.76566E+16
3 4.84614E+16 4.84614E+16 4.84614E+16 4.84614E+16 4.84614E+16 4.84614E+16 4.84614E+16 4.84614E+16 4.84614E+16
2 4.90017E+16 4.90017E+16 4.90017E+16 4.90017E+16 4.90017E+16 4.90017E+16 4.90017E+16 4.90017E+16 4.90017E+16
1 4.92729E+16 4.92729E+16 4.92729E+16 4.92729E+16 4.92729E+16 4.92729E+16 4.92729E+16 4.92729E+16 4.92729E+16
...
REGION ZONE ZONE VOLUME TOTAL FLUX PEAK FLUX (1) TOTAL FAST FLUX PEAK FAST FLUX(1)
NO. NAME NO. NAME (CC) (NEUTRON-CM/SEC) (NEUTRON/CM2-SEC) (NEUTRON-CM/SEC) (NEUTRON/CM2-SEC)
1 REGN1 1 REGN1 3.14159E+02 8.39223E+18 4.92729E+16 0.00000E+00 0.00000E+00
2 REGN2 2 REGN2 6.59734E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
TOTALS 3.80133E+02 8.39223E+18 4.92729E+16 0.00000E+00 0.00000E+00

```

Figure 3-9. REBUS-PC Verification Test #4 Output Excerpt

With the preceding results, this verification test demonstrates the following capabilities:

- Capability 1, as it compares an analytic eigenvalue based reference solution with the underlying finite difference approximation in REBUS-PC.
- Capability 6, as it demonstrates the application of internal black boundary conditions compared against an analytic reference solution.

This verification test provides no additional accuracy information on capabilities 4, 5, or 7 from verification test #3, as the identical analytical solution is applied.

3.6 Verification Test #5

Verification test #5 is effectively identical to verification test #3 but with extrapolated boundary conditions in the axial direction. Figure 3-10 provides the truncated input, where the major changes from test #3 are on the A.NIP3 card types 04 and 05, as indicated. This verification test is a true 2-D verification as there is no variance in the solution for the θ direction. The reference solution was obtained by independent implementation of the finite difference methodology with the Matlab program [12]. By executing the Matlab program, the same eigenvalue and flux solution are obtained as those found in the REBUS-PC, where no error exists due to the identical methodology and meshing being implemented. The output excerpt is provided in Figure 3-11 to record the eigenvalue and partial flux solution details obtained for the stated discrete math problem.

This verification test demonstrates the following capabilities:

- Capability 1, as it compares an analytic eigenvalue based reference solution with the underlying finite difference approximation in REBUS-PC.
- Capability 5, as it demonstrates the use of extrapolated boundary conditions in the R and Z directions.

This verification test provides no additional accuracy information on capabilities 4 or 7 from verification test #3.

```

UNFORM=A.DIF3D
01 *****                      1GTRZ_hom Model                      *****
02      10000 11000000
03          0      0      0      0      50
04          1      1      1      00 010      10      110      0      0      0      0
05              1.0E-07      1.0E-07      1.0E-07
06              1.0      1.0E-05      1.0E-05      10.0E+6
DATASET=A.HMG4C
01      TURN OFF HMG4C EDITS
02      60000      0      1      0      0      0
DATASET=A.NIP3
01 *****                      1GTRZ_hom Model                      *****
02              0      1 37000      0 750000 10000      0      0      0      0
03              66
04              6      6      3      4      4      4
05              YU 0.5
05              ZL 0.5
05              ZU 0.5
06      HMPREG 0.000000E+00 7.85400E-01      0      20 0.000000E+00 1.00000E+01
09              X      9 7.85400E-01
09              Y     10 1.00000E+01
09              Z     20 2.00000E+01
...

```

Figure 3-10. Truncated Input for Verification Test #5

...	OUTER ITERATIONS COMPLETED AT ITERATION 14, ITERATIONS HAVE CONVERGED									
0	K-EFFECTIVE = 0.97603431185									
...										
0	GROUP SUM OF	REAL FLUX FOR	K-EFF PROBLEM FOR PLANE	1 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)0	R-AXIS	THETA				
0	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA
	1	2	3	4	5	6	7	8	9	
10	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15
9	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15
8	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15
7	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15
6	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15
5	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15
4	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15
3	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15
2	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15
1	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15
0	GROUP SUM OF	REAL FLUX FOR	K-EFF PROBLEM FOR PLANE	2 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)	R-AXIS	THETA				
0	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA
	1	2	3	4	5	6	7	8	9	
10	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15	2.31749E+15
9	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15	3.62845E+15
8	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15	4.93118E+15
7	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15	6.18414E+15
6	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15	7.34684E+15
5	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15	8.38130E+15
4	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15	9.25345E+15
3	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15	9.93436E+15
2	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16	1.04014E+16
1	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16	1.06388E+16
...										
0	GROUP SUM OF	REAL FLUX FOR	K-EFF PROBLEM FOR PLANE	20 WITH ENERGY RANGE (EV) =(0.000E+00,1.000E+07)	R-AXIS	THETA				
0	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA
	1	2	3	4	5	6	7	8	9	
10	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15	1.51249E+15
9	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15	2.36808E+15
8	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15	3.21829E+15
7	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15	4.03603E+15
6	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15	4.79486E+15
5	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15	5.46999E+15
4	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15	6.03919E+15
3	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15	6.48358E+15
2	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15	6.78836E+15
1	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15	6.94335E+15

Figure 3-11. REBUS-PC Verification Test #5 Output Excerpt

3.7 Verification Tests #6, #7, and #8

Verification tests #6 through #8 are modifications of the input to demonstrate the impact of up-scattering iterations and Tchebychev acceleration. The base problem is the seven-group, 0-D benchmark which has a known analytical solution, described earlier as 7GTRZ_hom. Table 3-6 shows the setup differences between the three verification tests along with the resulting eigenvalue and number of fission source iterations used. Because the inputs all have the same setup on A.DIF3D card type 06, as shown in the verification test #6 input excerpt in Figure 3-12, the number of inner iterations used in each up-scatter iteration of each fission source (outer) iteration is identical between the three verification tests.

Table 3-6. Verification Test #6, #7, and #8 Setup Differences and Results

Mesh No.	Verification Test #6	Verification Test #7	Verification Test #8
Tchebychev Acceleration	No	No	Yes
Up-scatter Iterations	1	3	3
k-effective	1.583837 37224	1.583837 37252	1.583837 36899
Fission Source Iterations	23	15	12

DATASET=A.DIF3D											
01	*****	7GTRZ_hom Model						*****			
02	10000	11000									
03	0	0	1	0	500	0	1				
04	1	1	1	00	010	10	110	0	0	0	0
05		1.0E-07		1.0E-07		1.0E-07					
06		1.0		0.001		0.04		10.0E+6			
Test #07 and #08 type 03 alternative inputs											
	0	0	1	0	500	0	3				
	0	0	0	0	500	0	3				
DATASET=A.NIP3											
01	*****	7GTRZ_hom Model						*****			
02		0	1	37000	0	750000	10000	0	0	0	0
03		66									
04		3	3	3	3	3	3				
06	HMREG	0.00000E+00	7.85400E-01		0	20	0.00000E+00	2.00000E+01			
09	X	9	7.85400E-01								
09	Y	20	2.00000E+01								
09	Z	20	2.00000E+01								
13	MEAT1	U35A_0	2.2518E-03	U38A_0	9.0341E-03	PU9A_0	1.0000E-20				
13	MEAT1	LFPA_0	1.0000E-20	O16B_0	1.0000E-20						
13	MODA	H01A_0	6.6691E-02	O16A_0	3.3346E-02						
14	MIXA	MEAT1	3.6857E-01	MODA	6.3143E-01						
14	FUEL1	MIXA	1.0								
15	FUEL1	HMREG									
...											

Figure 3-12. Truncated Input for Verification Test #6

Because this is a homogeneous problem, the code will not stop until it reaches the same solution as the fission source error is directly related to the flux error everywhere in the domain. However, this verification test is sufficient proof that using up-scattering iterations impacts the solution scheme as anticipated. In Table 3-6, one can see that the software requires more fission source iterations to

converge the problem when 1 up-scattering iterations is used relative to using three (tests #7 and #8). Similarly, Tchebychev acceleration (test #8) reduces the total number of iterations required to complete the calculation. With regard to the differences in k-effective, one can see that they are within the 1.0E-7 convergence setting applied to the eigenvalue in Figure 3-12 on card type 06 of the A.DIF3D input.

These verification tests demonstrates the following capability:

- Capability 10, as it compares an analytic eigenvalue solution with results obtained with REBUS-PC. An additional test on a large scale problem is suggested for further confidence.

These tests provide no additional verification of the remaining capabilities.

3.8 Verification Tests #9, #10, and #11

Verification tests #9 through #11 are focused on the seven-group 3-D problem shown earlier in Figure 2-4 to further support capabilities #1, #4, #5, #7, and #10. Because of the complex solution capability, a modified input approach is used to verify the accuracy of the solution scheme. For any given mesh refinement, a new mathematically solvable system can be defined by taking the solution and converting it to a fixed source scheme. In this regard, the flux solution obtained from DIF3D in the standard eigenvalue mode of verification test #10 was used to turn the fission source into a fixed source input and solve the problem again using a steady state fixed source driven algorithm in verification test #9. Verification test #11 uses a modified input setup specifically needed for verifying capability 1.

The fixed-source problem solved in DIF3D can be formulated as:

$$M\vec{\phi} = F\vec{\phi} + \vec{S}_{ex}, \quad (6)$$

where $\vec{\phi}$ is the multi-group flux vector, $\vec{S}_{ex}$ is the independent external source distribution, M is the migration and loss operator, and F is the fission production operator. With an arbitrarily manufactured flux distribution $\vec{\phi}^m$, the corresponding independent source distribution can be deduced as:

$$\vec{S}_{ex} = M\vec{\phi}^m - F\vec{\phi}^m. \quad (7)$$

The source distribution can then be used in the DIF3D fixed-source calculation to test whether the resulting DIF3D flux solution $\vec{\phi}$ is identical to the original manufactured flux distribution $\vec{\phi}^m$. To simplify the preparation of the manufactured solution, the solution from verification test #10 was used to construct the source in equation 7. The resulting flux distribution $\vec{\phi}^e$ was chosen as the manufactured solution (i.e. $\vec{\phi}^m = \vec{\phi}^e$). The external source distribution in equation 7 was computed using a MATLAB script and the macroscopic cross sections printed out by the REBUS-PC software. The deduced independent source distribution was written in a FIXSRC file for input which is stored in the repository.

To understand the input differences, the input excerpts of verification test #9 are presented in Figure 3-13 showing the only sections of input that change relative to verification test #10 in Figure 3-14. As can be seen, only the DATASET card input and fixed source switch in A.DIF3D change. To show the output similarities and differences, output excerpts are provided for tests #9 and #10 in Figure 3-15 (similarities in the REBUS-PC output) and Figure 3-16 (differences in the output).

```

BLOCK=OLD
DATASET=ISOTXS
DATASET=FIXSRC
BLOCK=STP027
UNFORM=A.DIF3D
01 ***** 7GTRZ_het Model *****
02      10000 11000000
03      1      0      0 4500      50
04      1      1      1      00 010      10      111      0      0      0      0
05      1.0E-07      1.0E-07      1.0E-07
06      1.0      1.0E-05      1.0E-05      10.0E+6
...
DATASET=A.NIP3
01 ***** 7GTRZ_het Model *****
02      0      1 37000      0 750000 10000      0      0      0      0
03      66
04      6      6      3      4      4      4
05      YU 0.5
05      ZL 0.5
05      ZU 0.5
06      CORE1 0.00000E+00 7.85400E-01      0      20 0.00000E+00 1.00000E+01
06      CORE2 7.85400E-01 1.57080E+00      0      20 0.00000E+00 1.00000E+01
06      RFLT1 0.00000E+00 7.85400E-01      0      20 1.00000E+01 2.00000E+01
06      RFLT2 7.85400E-01 1.57080E+00      0      20 1.00000E+01 2.00000E+01
07      FUELX CORE1 CORE2
07      TCORE CORE1 CORE2 RFLT1 RFLT2
09      X      9 7.85400E-01
09      X      9 1.57080E+00
09      Y     10 1.00000E+01
09      Y     10 2.00000E+01
09      Z     20 2.00000E+01
13      MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 PU9A_0 1.0000E-20
13      MEAT1 LFPA_0 1.0000E-20 O16B_0 1.0000E-20
13      MODA H01A_0 6.6691E-02 O16A_0 3.3346E-02
14      MIXA MEAT1 3.6857E-01 MODA 6.3143E-01
14      MIXB MEAT1 3.0857E-01 MODA 6.9143E-01
14      FUEL1 MIXA 1.0
14      FUEL2 MIXB 1.0
15      FUEL1 CORE1
15      FUEL2 CORE2
14      REFLT H01A_0 6.6691E-02 O16A_0 3.3346E-02
15      REFLT RFLT1
15      REFLT RFLT2
...

```

Figure 3-13. Truncated Input for Verification Test #9

```

BLOCK=OLD
DATASET=ISOTXS
BLOCK=STP027
...
UNFORM=A.DIF3D
01 ***** 7GTRZ_het Model *****
02      10000 11000000
03      0      0      0 4500      50
04      1      1      1      00 010      10      111      0      0      0      0
05      1.0E-07      1.0E-07      1.0E-07
06      1.0      1.0E-05      1.0E-05      10.0E+6
...

```

Figure 3-14. Truncated Input for Verification Test #10

Verification Test #9									
...	1	IPROBT	0/1	EIGENVALUE/FIXED SOURCE PROBLEM					
	0	ISOLNT	0/1	REAL/ADJOINT SOLUTION					
	0	IXTRAP	0/1	YES/NO CHEBYSHEV OUTER ACCELERATION					
	0	IRSTRT	0/1	NO/YES THIS IS A RESTART					
	0	IOSAVE	0/1	NO/YES BYPASS LAST CONCURRENT INNER ITERATION PASS IN GROUPS BELOW THE LAST PASS THRESHOLD					
	0	IOMEG	0/1	NO/YES ASYMPTOTIC EXTRAPOLATION DURING THE OPTIMUM OVERRELAXATION FACTOR ESTIMATION ITERATIONS					
...									
0	OUTER	REL. POINT	REL. SUM	EIGENVALUE	POLY.	SPEC. RAD.	SPEC. RAD.		TOTAL
	IT. NO.	ERROR	ERROR	CHANGE	ORDER	USED	ESTIMATED	K-EFFECTIVE	FISSION SOURCE
0	28	6.018997E-07	3.832083E-07	0.000000E+00	2	9.370057E-01	7.662016E-01	1.00000000E+00	7.72863070E+17
0	29	4.485614E-07	3.325875E-07	0.000000E+00	3	9.370057E-01	9.086408E-01	1.00000000E+00	7.72863469E+17
0	30	3.570210E-07	3.202435E-07	0.000000E+00	4	9.370057E-01	9.441788E-01	1.00000000E+00	7.72863700E+17
0	31	2.268336E-07	1.602635E-07	0.000000E+00	1	9.441788E-01	5.004426E-01	1.00000000E+00	7.72863735E+17
0	32	2.105298E-07	1.465765E-07	0.000000E+00	2	9.441788E-01	9.549150E-01	1.00000000E+00	7.72863736E+17
0	33	1.457418E-07	9.392586E-08	0.000000E+00	3	9.441788E-01	9.297550E-01	1.00000000E+00	7.72863760E+17
0	34	1.074029E-07	7.227955E-08	0.000000E+00	4	9.441788E-01	9.446820E-01	1.00000000E+00	7.72863789E+17
0	35	9.396232E-08	6.474451E-08	0.000000E+00	1	9.446820E-01	8.957515E-01	1.00000000E+00	7.72863799E+17
0	OUTER ITERATIONS COMPLETED AT ITERATION 35, ITERATIONS HAVE CONVERGED								
...									
Verification Test #10									
...	0	IPROBT	0/1	EIGENVALUE/FIXED SOURCE PROBLEM					
	0	ISOLNT	0/1	REAL/ADJOINT SOLUTION					
	0	IXTRAP	0/1	YES/NO CHEBYSHEV OUTER ACCELERATION					
	0	IRSTRT	0/1	NO/YES THIS IS A RESTART					
	0	IOSAVE	0/1	NO/YES BYPASS LAST CONCURRENT INNER ITERATION PASS IN GROUPS BELOW THE LAST PASS THRESHOLD					
	0	IOMEG	0/1	NO/YES ASYMPTOTIC EXTRAPOLATION DURING THE OPTIMUM OVERRELAXATION FACTOR ESTIMATION ITERATIONS					
...									
0	OUTER	REL. POINT	REL. SUM	EIGENVALUE	POLY.	DOM. RATIO	DOM. RATIO		
	IT. NO.	ERROR	ERROR	CHANGE	ORDER	USED	ESTIMATED	K-EFFECTIVE	
0	17	3.256490E-06	3.530648E-06	1.663527E-06	2	6.277783E-01	7.520596E-01	6.35447036E-01	
0	18	4.638986E-07	6.241755E-07	1.195276E-06	3	6.277783E-01	6.250962E-01	6.35448231E-01	
0	19	9.991518E-07	8.897229E-07	5.685850E-07	4	6.277783E-01	7.355684E-01	6.35448799E-01	
0	20	3.995519E-07	4.548968E-07	2.695249E-07	1	7.355684E-01	5.112795E-01	6.35449069E-01	
0	21	2.887825E-07	2.791872E-07	1.929800E-07	2	7.355684E-01	7.557989E-01	6.35449262E-01	
0	22	8.168624E-08	6.330316E-08	8.724450E-08	3	7.355684E-01	7.051897E-01	6.35449349E-01	
0	OUTER ITERATIONS COMPLETED AT ITERATION 22, ITERATIONS HAVE CONVERGED								
0	K-EFFECTIVE = 0.63544934914								

Figure 3-15. REBUS-PC Verification Tests #9 and #10 Output Differences

Verification Test #9											
...	REGION NO.	ZONE NAME	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC) (2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION	
	1	CORE1	1	CORE1	7.85400E+02	1.00000E+00	5.07613E+06	6.46311E+03	2.44247E+04	5.07613E-01	
	2	CORE2	2	CORE2	7.85400E+02	1.00000E+00	4.86147E+06	6.18980E+03	2.19016E+04	4.86147E-01	
	3	RFLT1	3	RFLT1	2.35620E+03	1.00000E+00	3.10810E+04	1.31912E+01	3.12392E+01	3.10810E-03	
	4	RFLT2	4	RFLT2	2.35620E+03	1.00000E+00	3.13237E+04	1.32942E+01	3.14642E+01	3.13237E-03	
	TOTALS				6.28320E+03	0.00000E+00	1.00000E+07	1.59155E+03	2.44247E+04	1.53465E+01	1.00000E+00
...											
0	REAL FLUX FOR SOURCE PROBLEM FOR PLANE 1 FOR GROUP 1 WITH ENERGY RANGE (EV) =(8.210E+05,1.000E+07)										
0	R-AXIS	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	
		1	2	3	4	5	6	7	8	9	
	20	7.79972E+13	7.81111E+13	7.82028E+13	7.82617E+13	7.82820E+13	7.82617E+13	7.82028E+13	7.81111E+13	7.79972E+13	
	19	1.01940E+14	1.02095E+14	1.02220E+14	1.02299E+14	1.02327E+14	1.02299E+14	1.02220E+14	1.02095E+14	1.01940E+14	
	18	1.34369E+14	1.34588E+14	1.34762E+14	1.34873E+14	1.34911E+14	1.34873E+14	1.34762E+14	1.34588E+14	1.34369E+14	
	17	1.78116E+14	1.78433E+14	1.78683E+14	1.78841E+14	1.78895E+14	1.78841E+14	1.78683E+14	1.78433E+14	1.78116E+14	
	16	2.37027E+14	2.37495E+14	2.37860E+14	2.38088E+14	2.38165E+14	2.38088E+14	2.37860E+14	2.37495E+14	2.37027E+14	
	15	3.16329E+14	3.17036E+14	3.17576E+14	3.17908E+14	3.18018E+14	3.17908E+14	3.17576E+14	3.17036E+14	3.16329E+14	
	14	4.23140E+14	4.24235E+14	4.25044E+14	4.25527E+14	4.25686E+14	4.25527E+14	4.25044E+14	4.24235E+14	4.23140E+14	
...											
Verification Test #10											
...	REGION NO.	ZONE NAME	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC) (2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION	
	1	CORE1	1	CORE1	7.85400E+02	1.00000E+00	5.07613E+06	6.46311E+03	2.44247E+04	5.07613E-01	
	2	CORE2	2	CORE2	7.85400E+02	1.00000E+00	4.86147E+06	6.18980E+03	2.19016E+04	4.86147E-01	
	3	RFLT1	3	RFLT1	2.35620E+03	1.00000E+00	3.10810E+04	1.31912E+01	3.12392E+01	3.10810E-03	
	4	RFLT2	4	RFLT2	2.35620E+03	1.00000E+00	3.13237E+04	1.32942E+01	3.14642E+01	3.13237E-03	
	TOTALS				6.28320E+03	0.00000E+00	1.00000E+07	1.59155E+03	2.44247E+04	1.53465E+01	1.00000E+00
...											
0	REAL FLUX FOR K-EFF PROBLEM FOR PLANE 1 FOR GROUP 1 WITH ENERGY RANGE (EV) =(8.210E+05,1.000E+07)										
0	R-AXIS	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	THETA	
		1	2	3	4	5	6	7	8	9	
	20	7.79972E+13	7.81111E+13	7.82027E+13	7.82617E+13	7.82820E+13	7.82617E+13	7.82027E+13	7.81111E+13	7.79972E+13	
	19	1.01940E+14	1.02095E+14	1.02220E+14	1.02299E+14	1.02327E+14	1.02299E+14	1.02220E+14	1.02095E+14	1.01940E+14	
	18	1.34369E+14	1.34588E+14	1.34762E+14	1.34873E+14	1.34911E+14	1.34873E+14	1.34762E+14	1.34588E+14	1.34369E+14	
	17	1.78116E+14	1.78433E+14	1.78683E+14	1.78841E+14	1.78895E+14	1.78841E+14	1.78683E+14	1.78433E+14	1.78116E+14	
	16	2.37027E+14	2.37495E+14	2.37860E+14	2.38088E+14	2.38165E+14	2.38088E+14	2.37860E+14	2.37495E+14	2.37027E+14	
	15	3.16329E+14	3.17036E+14	3.17576E+14	3.17907E+14	3.18018E+14	3.17907E+14	3.17576E+14	3.17036E+14	3.16329E+14	
	14	4.23140E+14	4.24235E+14	4.25044E+14	4.25527E+14	4.25686E+14	4.25527E+14	4.25044E+14	4.24235E+14	4.23140E+14	

Figure 3-16. REBUS-PC Verification Tests #9 and #10 Output Similarities

Looking at Figure 3-15, one can clearly see that the solution algorithm has switched from a fixed source case in test #9 to a flux solution in test #10. The iterative eigenvalue convergence routine in test #10 is replaced by the fixed source driven sub-critical system algorithm in #9, which is also visible in Figure 3-15. REBUS-PC Verification Tests #9 and #10 Output Differences. Looking at the flux solution excerpts from these tests in Figure 3-16 one finds that the solution is identical to six significant digits. Further inspection of the remaining flux and power output demonstrates that the REBUS-PC solutions between #09 and #10 are indistinguishable.

As an additional test of specific input handling, the input of verification tests #9 and #10 were modified to that seen in verification test #11, as shown in Figure 3-17. A comparison of the input excerpt for verification test #9 shows that two card type 15 inputs in A.NIP3 were replaced with a single card type 15 input in verification test #11. The primary difference, of course, is that the new card type 15 uses the area specification to assign a composition rather than the region specification. Inspection of the output of verification test #11 shows it is an identical result to that of #10.

```

BLOCK=OLD
DATASET=ISOTXS
BLOCK=STP027
...
DATASET=A.NIP3
01 ***** 7GTRZ_het Model *****
02          0      1 37000      0 750000 10000      0      0      0      0
03          66
04          6      6      3      4      4      4
05          YU 0.5
05          ZL 0.5
05          ZU 0.5
06 CORE1 0.00000E+00 7.85400E-01      0      20 0.00000E+00 1.00000E+01
06 CORE2 7.85400E-01 1.57080E+00      0      20 0.00000E+00 1.00000E+01
06 RFLT1 0.00000E+00 7.85400E-01      0      20 1.00000E+01 2.00000E+01
06 RFLT2 7.85400E-01 1.57080E+00      0      20 1.00000E+01 2.00000E+01
07 FUELX CORE1 CORE2
07 REFLX RFLT1 RFLT2
07 TCORE CORE1 CORE2 RFLT1 RFLT2
09          X      9 7.85400E-01
09          X      9 1.57080E+00
09          Y     10 1.00000E+01
09          Y     10 2.00000E+01
09          Z     20 2.00000E+01
13          MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 PU9A_0 1.0000E-20
13          MEAT1 LFPA_0 1.0000E-20 O16B_0 1.0000E-20
13          MODA H01A_0 6.6691E-02 O16A_0 3.3346E-02
14          MIXA MEAT1 3.6857E-01 MODA 6.3143E-01
14          MIXB MEAT1 3.0857E-01 MODA 6.9143E-01
14          FUEL1 MIXA 1.0
14          FUEL2 MIXB 1.0
15          FUEL1 CORE1
15          FUEL2 CORE2
14          REFLT H01A_0 6.6691E-02 O16A_0 3.3346E-02
15          REFLT REFLX
...

```

Figure 3-17. Truncated Input for Verification Test #11

These three verification tests demonstrate the following capability:

- Capability 1, as it compares the solution for identical, but alternative 3-D θ -R-Z models

These verification tests provide no additional verification of capabilities 4, 5, 7, or 10, as the details of the solution were not checked against an analytic solution or modified to test the impact of input changes. They also provide no additional verification for the remaining capabilities.

3.9 Supplemental Verification of Capabilities 1, 4, and 5

The preceding analytic solution only considers the radial aspect of the domain and effectively uses reflected boundary conditions in the axial and θ direction, eliminating the potential for gradients. To complete the test, a discrete math problem validation case is chosen that is testable using REBUS-PC. The primary problem with obtaining an analytic solution to the neutron transport or diffusion equation is the scattering and fission operators which depend upon the flux solution itself and spatial variations in the cross sections. If those cross sections become piece-wise constants, then the analytic solution quickly devolves into a very complex infinite series expansion. To overcome this the fixed source solution capability is used to demonstrate the remaining spatial fidelity by zeroing out the fission and scattering cross sections. A fixed source is introduced with constant cross sections over the whole domain to arrive at the differential equation

$$\bar{\nabla} D \bar{\nabla} \phi(\theta, r, z) + \Sigma_a \cdot \phi(\theta, r, z) = S(\theta, r, z) \quad (8)$$

Under certain circumstances and boundary conditions, this equation can have a manageable analytic solution which can be used to test REBUS-PC. In this case, an analytic solution is not required, as merely defining a flux solution that is consistent with the differential equation is sufficient to demonstrate the finite difference solver imbedded in REBUS-PC. Of particular interest for this work is that the differential equation, for certain sources, produces a relatively smooth solution that can be used to verify the θ and Z approximations, as the previous tests have already verified the R direction approximation. For simplicity, the boundary conditions impose a zero flux condition at the domain interfaces at $r=R$, $z=0$, $z=Z$, and periodic boundary condition in θ , such that the following holds:

$$\begin{aligned} \phi(\theta, r, 0) = 0, \quad \phi(\theta, R, z) = 0, \quad \phi(\theta, r, Z) = 0, \\ \left. \frac{\partial}{\partial r} \phi(\theta, r, 0) \right|_{r=0} = 0, \quad \phi(0, r, z) = \phi(2 \cdot \pi, r, z) \end{aligned} \quad (9)$$

Because REBUS-PC cannot model an explicit spatially continuous source, the input must be progressively refined to show convergence towards a reference solution. To satisfy the above boundary conditions the flux solution can have the form:

$$\phi(\theta, r, z) = (r^3 - r^4) \cdot \cos(r \cdot 0.5 \cdot \pi) \cdot (1 + 0.5 \cdot \cos \theta) \sin(\pi z) \quad r \in 0, 1 \quad z \in 0, 1 \quad \theta \in 0, 2\pi \quad (10)$$

The source for this system is obtained by substituting the flux solution into the differential equation:

$$S(\theta, r, z) = D \cdot \left[\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial^2 \theta} + \frac{\partial^2}{\partial^2 z} \right] \phi(\theta, r, z) + \Sigma_a \cdot \phi(\theta, r, z), \quad (11)$$

where $D=0.05$ cm and $\Sigma=2$ cm⁻¹ are chosen, noting that negative source moments are not an issue for this mathematical problem. Because the functional representation of the source is very large, a spatial flux profile of the source is provided along with the flux solution in Figure 3-18. A quick inspection of equation 10 and the plots of Figure 3-18 shows that the solution satisfies the boundary conditions defined in equation 9, and thus should be solvable by DIF3D.

The source is prepared for REBUS-PC by computing the average source over the volume of each REBUS-PC mesh and creating the appropriate card inputs for A.NIP3. The reference solution is obtained similarly by averaging the reference flux solution over each mesh. A MathCAD [10] program was used to prepare the source and reference flux solution appropriate for REBUS-PC. Because the

solution data is extensive, the accuracy of the solution with respect to mesh refinement is considered. Figure 3-19 shows the radial flux profile ($\theta \times R \times Z$) at $Z=0.5$ for three different meshes in REBUS-PC along with the reference solution. As can be seen, the REBUS-PC profile converges to the reference solution as the number of mesh are increased. The appearance of the reference flux profiles differ between Figure 3-19 and Figure 3-18 only because of the use of different plotting software and choice of color tables.

Figure 3-18. Reference Flux and Source Profiles for Supplemental Test Problem

Figure 3-19. REBUS-PC Flux Profiles for Supplemental Test Problem

To better illustrate the agreement between REBUS-PC and the reference solution, Figure 3-20 shows the θ flux trace at $Z=0.5$ and $R=0.75$ and the relative error results obtained using REBUS-PC. This particular trace was shown as it is part of both Figure 3-19 and Figure 3-18 and shows that the REBUS-PC calculated result has very little error. Even for the coarse mesh result, the relative error is still under 0.5%. As the mesh is refined, the error drops to less than 0.005%. It is important to note that the REBUS-PC flux solution is not accurate at all points, as REBUS-PC still produces negative flux solutions near the boundary and center of the domain due to insufficient mesh refinement to handle

the gradients. Overall, however, this problem fully demonstrates that the θ -R-Z capability of REBUS-PC is functioning properly given the stated boundary conditions. This supplemental benchmark problem was not added to the verification test suite, as the remaining verification tests that demonstrate the STRZ geometry are sufficient to show that the flux solution capability is working properly, given that this demonstration was done, and track any issues that occur with the solution accuracy as the software progresses.

Figure 3-20. REBUS-PC Flux Error Profiles for Supplemental Test Problem

3.10 Verification Tests #12, #13, and #14

Verification tests #12 through #14 are focused on checking that the input is properly processed by the REBUS-PC software. The STRZ benchmark geometry defined earlier in Figure 2-2 is the base geometry input for all three of these verification tests. The STRZ geometry is complex and contains seven depletion steps with control rod movements. The main purpose of verification test #12 is to define the base solution for the STRZ benchmark and verify that the complicated geometry details of the STRZ benchmark are properly processed by DIF3D. Most of the verification can be done by looking at the processed geometry output of DIF3D. Starting with Figure 3-21, the number of regions, zones, and meshing required to define the STRZ benchmark can be verified to be consistent with the input. The region and zone map output of REBUS-PC, an excerpt of which is shown in Figure 3-22, can be compared to verify that DIF3D assigned the correct regions and zones to the spatial locations in STRZ. Finally, verification test #12 is used to verify the power distribution and the TYPE13.BCD file output.

The region map in Figure 3-22 was produced by REBUS-PC by enabling the third and fourth input flags on card type 04 in A.DIF3D. In the region map, the numbers on the first row denote the mesh index in the theta-direction (i.e., the azimuthal direction) and the numbers in the first column denote the mesh index in R-direction (i.e. the radial direction). Star symbols (*) mark the region boundaries. The numbers other than the mesh indices refer to a region that contains the specific mesh. In another section of output, these region numbers are linked to the region names provided, and, via cross

checking, the map shown can be shown to match the input specification. The region and area volumes were also checked by comparing the values given in the output and those calculated using Microsoft Excel [13]. The manual check is provided for the θ mesh boundaries in Table 3-7, the R mesh boundaries in Table 3-8 and the Z mesh boundaries in Table 3-9. This result is as expected as the mesh boundaries computed and reported by DIF3D are identical to those calculated in the Excel document.

--- MODEL DESCRIPTION ---		
15	IGOM	GEOMETRY TYPE, THETA-R-Z
10	NZONE	NO. OF ZONES (COMPOSITIONS)
230	NREG	NO. OF REGIONS
1	NZCL	NO. OF ZONE CLASSIFICATIONS
8	NCINTI	NO. OF 1ST DIMENSION COARSE MESH INTERVALS
15	NCINTJ	NO. OF 2ND DIMENSION COARSE MESH INTERVALS
6	NCINTK	NO. OF 3RD DIMENSION COARSE MESH INTERVALS
72	NINTI	NO. OF 1ST DIMENSION FINE MESH INTERVALS
39	NINTJ	NO. OF 2ND DIMENSION FINE MESH INTERVALS
28	NINTK	NO. OF 3RD DIMENSION FINE MESH INTERVALS
3	IMB1	FIRST BOUNDARY CONDITION, FIRST DIMENSION, PERIODIC, OPPOSITE FACE
3	IMB2	LAST BOUNDARY CONDITION, FIRST DIMENSION, PERIODIC, OPPOSITE FACE
1	JMB1	FIRST BOUNDARY CONDITION, SECOND DIMENSION, REFLECTED
2	JMB2	LAST BOUNDARY CONDITION, SECOND DIMENSION, EXTRAPOLATED
1	KMB1	FIRST BOUNDARY CONDITION, THIRD DIMENSION, REFLECTED
2	KMB2	LAST BOUNDARY CONDITION, THIRD DIMENSION, EXTRAPOLATED
1	NBS	NO. OF BUCKLING SPECIFICATIONS
1	NBCS	NO. OF CONSTANTS FOR EXTERNAL BOUNDARIES
1	NIBCS	NO. OF CONSTANTS FOR INTERNAL BOUNDARIES
0	NZWBB	NO. OF BLACKNESS THEORY ZONES
0	NRASS	0/1, REGION ASSIGNMENTS TO COARSE/FINE MESH

Figure 3-21. Model Descriptions in REBUS-PC Standard Output

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
39	*	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
38	*	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
37	*	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
36	*	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
35	*	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
34	*	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
33	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
32	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
31	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
30	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
29	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
28	*	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	225	225
27	*	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	225	225
26	*	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
25	*	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
24	*	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
23	*	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19
22	*	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19
21	*	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136
20	*	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136	136

Figure 3-22. Region Map Output Table Excerpt from REBUS-PC for Verification Test #12

Table 3-7. Verification Test #12 Check of the θ Mesh Boundaries

No.	REBUS-PC	Excel	Diff.	No.	REBUS-PC	Excel	Diff.
1	0.00000E+00	0.00000E+00	0.00000E+00	38	3.22886E+00	3.22886E+00	0.00000E+00
2	8.72664E-02	8.72664E-02	0.00000E+00	39	3.31612E+00	3.31612E+00	0.00000E+00
3	1.74533E-01	1.74533E-01	0.00000E+00	40	3.40339E+00	3.40339E+00	0.00000E+00
4	2.61799E-01	2.61799E-01	0.00000E+00	41	3.49066E+00	3.49066E+00	0.00000E+00
5	3.49066E-01	3.49066E-01	0.00000E+00	42	3.57792E+00	3.57792E+00	0.00000E+00
6	4.36332E-01	4.36332E-01	0.00000E+00	43	3.66519E+00	3.66519E+00	0.00000E+00
7	5.23599E-01	5.23599E-01	0.00000E+00	44	3.75246E+00	3.75246E+00	0.00000E+00
8	6.10865E-01	6.10865E-01	0.00000E+00	45	3.83972E+00	3.83972E+00	0.00000E+00
9	6.98132E-01	6.98132E-01	0.00000E+00	46	3.92699E+00	3.92699E+00	0.00000E+00
10	7.85398E-01	7.85398E-01	0.00000E+00	47	4.01426E+00	4.01426E+00	0.00000E+00
11	8.72665E-01	8.72665E-01	0.00000E+00	48	4.10152E+00	4.10152E+00	0.00000E+00
12	9.59932E-01	9.59932E-01	0.00000E+00	49	4.18879E+00	4.18879E+00	0.00000E+00
13	1.04720E+00	1.04720E+00	0.00000E+00	50	4.27606E+00	4.27606E+00	0.00000E+00
14	1.13447E+00	1.13447E+00	0.00000E+00	51	4.36332E+00	4.36332E+00	0.00000E+00
15	1.22173E+00	1.22173E+00	0.00000E+00	52	4.45059E+00	4.45059E+00	0.00000E+00
16	1.30900E+00	1.30900E+00	0.00000E+00	53	4.53786E+00	4.53786E+00	0.00000E+00
17	1.39627E+00	1.39627E+00	0.00000E+00	54	4.62512E+00	4.62512E+00	0.00000E+00
18	1.48353E+00	1.48353E+00	0.00000E+00	55	4.71239E+00	4.71239E+00	0.00000E+00
19	1.57080E+00	1.57080E+00	0.00000E+00	56	4.79966E+00	4.79966E+00	0.00000E+00
20	1.65807E+00	1.65807E+00	0.00000E+00	57	4.88692E+00	4.88692E+00	0.00000E+00
21	1.74533E+00	1.74533E+00	0.00000E+00	58	4.97419E+00	4.97419E+00	0.00000E+00
22	1.83260E+00	1.83260E+00	0.00000E+00	59	5.06146E+00	5.06146E+00	0.00000E+00
23	1.91986E+00	1.91986E+00	0.00000E+00	60	5.14872E+00	5.14872E+00	0.00000E+00
24	2.00713E+00	2.00713E+00	0.00000E+00	61	5.23599E+00	5.23599E+00	0.00000E+00
25	2.09439E+00	2.09439E+00	0.00000E+00	62	5.32326E+00	5.32326E+00	0.00000E+00
26	2.18166E+00	2.18166E+00	0.00000E+00	63	5.41052E+00	5.41052E+00	0.00000E+00
27	2.26892E+00	2.26892E+00	0.00000E+00	64	5.49779E+00	5.49779E+00	0.00000E+00
28	2.35619E+00	2.35619E+00	0.00000E+00	65	5.58506E+00	5.58506E+00	0.00000E+00
29	2.44346E+00	2.44346E+00	0.00000E+00	66	5.67232E+00	5.67232E+00	0.00000E+00
30	2.53072E+00	2.53072E+00	0.00000E+00	67	5.75959E+00	5.75959E+00	0.00000E+00
31	2.61799E+00	2.61799E+00	0.00000E+00	68	5.84685E+00	5.84685E+00	0.00000E+00
32	2.70526E+00	2.70526E+00	0.00000E+00	69	5.93412E+00	5.93412E+00	0.00000E+00
33	2.79252E+00	2.79252E+00	0.00000E+00	70	6.02138E+00	6.02138E+00	0.00000E+00
34	2.87979E+00	2.87979E+00	0.00000E+00	71	6.10865E+00	6.10865E+00	0.00000E+00
35	2.96706E+00	2.96706E+00	0.00000E+00	72	6.19591E+00	6.19591E+00	0.00000E+00
36	3.05432E+00	3.05432E+00	0.00000E+00	73	6.28318E+00	6.28318E+00	0.00000E+00
37	3.14159E+00	3.14159E+00	0.00000E+00				

Table 3-8. Verification Test #12 Check of the R Mesh Boundaries

No.	REBUS-PC	Excel	Diff.	No.	REBUS-PC	Excel	Diff.
1	0.00000E+00	0.00000E+00	0.00000E+00	21	1.80522E+01	1.80522E+01	0.00000E+00
2	1.99471E+00	1.99471E+00	0.00000E+00	22	1.86825E+01	1.86825E+01	0.00000E+00
3	3.98942E+00	3.98942E+00	0.00000E+00	23	1.95464E+01	1.95464E+01	0.00000E+00
4	4.90275E+00	4.90275E+00	0.00000E+00	24	2.04102E+01	2.04102E+01	0.00000E+00
5	5.81607E+00	5.81607E+00	0.00000E+00	25	2.13235E+01	2.13235E+01	0.00000E+00
6	6.72940E+00	6.72940E+00	0.00000E+00	26	2.22369E+01	2.22369E+01	0.00000E+00
7	7.59325E+00	7.59325E+00	0.00000E+00	27	2.31502E+01	2.31502E+01	0.00000E+00
8	8.45710E+00	8.45710E+00	0.00000E+00	28	2.37775E+01	2.37775E+01	0.00000E+00
9	9.08739E+00	9.08739E+00	0.00000E+00	29	2.44047E+01	2.44047E+01	0.00000E+00
10	9.71768E+00	9.71768E+00	0.00000E+00	30	2.52990E+01	2.52990E+01	0.00000E+00
11	1.05815E+01	1.05815E+01	0.00000E+00	31	2.61932E+01	2.61932E+01	0.00000E+00
12	1.14454E+01	1.14454E+01	0.00000E+00	32	2.70875E+01	2.70875E+01	0.00000E+00
13	1.20757E+01	1.20757E+01	0.00000E+00	33	2.79817E+01	2.79817E+01	0.00000E+00
14	1.27060E+01	1.27060E+01	0.00000E+00	34	2.88760E+01	2.88760E+01	0.00000E+00
15	1.35699E+01	1.35699E+01	0.00000E+00	35	3.22093E+01	3.22093E+01	0.00000E+00
16	1.44337E+01	1.44337E+01	0.00000E+00	36	3.55427E+01	3.55427E+01	0.00000E+00
17	1.50640E+01	1.50640E+01	0.00000E+00	37	3.88760E+01	3.88760E+01	0.00000E+00
18	1.56942E+01	1.56942E+01	0.00000E+00	38	4.22093E+01	4.22093E+01	0.00000E+00
19	1.65581E+01	1.65581E+01	0.00000E+00	39	4.55427E+01	4.55427E+01	0.00000E+00
20	1.74219E+01	1.74219E+01	0.00000E+00	40	4.88760E+01	4.88760E+01	0.00000E+00

Table 3-9. Verification Test #12 Check of the Z Mesh Boundaries

No.	REBUS-PC	Excel	Diff.	No.	REBUS-PC	Excel	Diff.
1	0.00000E+00	0.00000E+00	0.00000E+00	21	3.00000E+01	3.00000E+01	0.00000E+00
2	2.00000E+00	2.00000E+00	0.00000E+00	22	3.50000E+01	3.50000E+01	0.00000E+00
3	4.00000E+00	4.00000E+00	0.00000E+00	23	4.00000E+01	4.00000E+01	0.00000E+00
4	6.00000E+00	6.00000E+00	0.00000E+00	24	4.50000E+01	4.50000E+01	0.00000E+00
5	8.00000E+00	8.00000E+00	0.00000E+00	25	4.75000E+01	4.75000E+01	0.00000E+00
6	1.00000E+01	1.00000E+01	0.00000E+00	26	5.00000E+01	5.00000E+01	0.00000E+00
7	1.20000E+01	1.20000E+01	0.00000E+00	27	5.50000E+01	5.50000E+01	0.00000E+00
8	1.40000E+01	1.40000E+01	0.00000E+00	28	6.00000E+01	6.00000E+01	0.00000E+00
9	1.60000E+01	1.60000E+01	0.00000E+00	29	6.50000E+01	6.50000E+01	0.00000E+00
10	1.80000E+01	1.80000E+01	0.00000E+00	30	7.00000E+01	7.00000E+01	0.00000E+00
11	2.00000E+01	2.00000E+01	0.00000E+00	31	7.50000E+01	7.50000E+01	0.00000E+00
12	2.20000E+01	2.20000E+01	0.00000E+00	32	8.00000E+01	8.00000E+01	0.00000E+00
13	2.40000E+01	2.40000E+01	0.00000E+00	33	8.50000E+01	8.50000E+01	0.00000E+00
14	2.60000E+01	2.60000E+01	0.00000E+00	34	9.00000E+01	9.00000E+01	0.00000E+00
15	2.80000E+01	2.80000E+01	0.00000E+00	35			

In addition to the mesh boundaries, the region and area volumes reported by REBUS-PC were computed using Excel which is reported in Table 3-10.. As was the case with the mesh boundary calculations, the region and area volumes are identical to those of REBUS-PC.

Table 3-10. Verification Test #12 Check of the Region and Area Volumes

Region/ Area No.	Region/ Area Name	Region/Area Volume (cc)		Diff.
		REBUS-PC	Excel	
1	UPSTR	3.64817E+04	3.64817E+04	0.00000E+00
2	WPOOL	5.57556E+05	5.57556E+05	0.00000E+00
3	FTRAP	1.50000E+03	1.50000E+03	0.00000E+00
4	STWLI	2.76799E+03	2.76799E+03	0.00000E+00
5	STWLO	1.12490E+04	1.12490E+04	0.00000E+00
6	REFLT	2.24530E+04	2.24530E+04	0.00000E+00
7	CL11E	1.03035E+02	1.03035E+02	0.00000E+00
8	CL11F	1.03035E+02	1.03035E+02	0.00000E+00
9	CL11G	1.03035E+02	1.03035E+02	0.00000E+00
10	CL12E	1.43586E+02	1.43586E+02	0.00000E+00
11	CL12F	1.43586E+02	1.43586E+02	0.00000E+00
12	CL12G	1.43586E+02	1.43586E+02	0.00000E+00
13	CL13E	1.84134E+02	1.84134E+02	0.00000E+00
14	CL13F	1.84134E+02	1.84134E+02	0.00000E+00
15	CL13G	1.84134E+02	1.84134E+02	0.00000E+00
16	CL14E	2.24681E+02	2.24681E+02	0.00000E+00
17	CL14F	2.24681E+02	2.24681E+02	0.00000E+00
18	CL14G	2.24681E+02	2.24681E+02	0.00000E+00
19	CL15E	2.65231E+02	2.65231E+02	0.00000E+00
20	CL15F	2.65231E+02	2.65231E+02	0.00000E+00
21	CL15G	2.65231E+02	2.65231E+02	0.00000E+00
127	FL11E	8.99703E+01	8.99703E+01	0.00000E+00
128	FL11F	8.99703E+01	8.99703E+01	0.00000E+00
129	FL11G	8.99703E+01	8.99703E+01	0.00000E+00
130	FL12E	1.19558E+02	1.19558E+02	0.00000E+00
131	FL12F	1.19558E+02	1.19558E+02	0.00000E+00
132	FL12G	1.19558E+02	1.19558E+02	0.00000E+00
133	FL13E	1.49132E+02	1.49132E+02	0.00000E+00
134	FL13F	1.49132E+02	1.49132E+02	0.00000E+00
135	FL13G	1.49132E+02	1.49132E+02	0.00000E+00
136	FL14E	1.78730E+02	1.78730E+02	0.00000E+00
137	FL14F	1.78730E+02	1.78730E+02	0.00000E+00
138	FL14G	1.78730E+02	1.78730E+02	0.00000E+00
223	BLDW1	9.37102E+01	9.37102E+01	0.00000E+00
224	FOLL1	9.37102E+01	9.37102E+01	0.00000E+00
225	BLAD1	1.21823E+03	1.21823E+03	0.00000E+00
226	HADL1	7.02826E+02	7.02826E+02	0.00000E+00
227	BLDW2	1.87419E+02	1.87419E+02	0.00000E+00
228	FOLL2	9.37096E+01	9.37096E+01	0.00000E+00
229	BLAD2	1.12452E+03	1.12452E+03	0.00000E+00
230	HADL2	7.02822E+02	7.02822E+02	0.00000E+00
231	BLDW3	9.37102E+01	9.37102E+01	0.00000E+00
232	FOLL3	9.37102E+01	9.37102E+01	0.00000E+00
233	BLAD3	1.21823E+03	1.21823E+03	0.00000E+00
234	HADL3	7.02826E+02	7.02826E+02	0.00000E+00
Areas				
1	FUELX	1.28974E+04	1.28974E+04	0.00000E+00
2	BLADE	4.68550E+03	4.68550E+03	0.00000E+00
3	BL&FL	1.75829E+04	1.75829E+04	0.00000E+00

The solution produced by STRZ uses many flux calculations to reach the end of the depletion calculation, as evident from the tabulated eigenvalue results in Table 3-11, which notably are identical for all three test cases.

Table 3-11. Verification Tests #12, #13, and #14 Eigenvalue Results

Time Point	Verification Test #12	Verification Test #13	Verification Test #14
0.00	1.07900	1.07900	1.07900
3.00	1.03321	1.03321	1.03321
3.00	1.03308	1.03308	1.03308
6.00	1.02766	1.02766	1.02766
6.00	1.02778	1.02778	1.02778
9.00	1.02282	1.02282	1.02282
9.00	1.02282	1.02282	1.02282
12.00	1.01797	1.01797	1.01797
12.00	1.01797	1.01797	1.01797
15.00	1.01323	1.01323	1.01323
15.00	1.01323	1.01323	1.01323
18.00	1.01030	1.01030	1.01030
18.00	1.01030	1.01030	1.01030
21.00	1.00752	1.00752	1.00752
21.00	1.00752	1.00752	1.00752
24.00	1.00531	1.00531	1.00531
24.00	1.00531	1.00531	1.00531
27.00	1.00244	1.00244	1.00244
27.00	1.00244	1.00244	1.00244
30.00	0.99859	0.99859	0.99859
30.00	0.99859	0.99859	0.99859

Because the output file for each case is quite extensive, only those pieces that are relevant to the actual verification being done are compared. In verification test #13 the free format usage is checked where verification test #12 was provided to REBUS-PC using the fixed format input. The main input difference is thus a simple formatting change of the input such that it no longer has the required column layout of a fixed format input as shown in Figure 3-23. As expected, the results are identical, as inferred by Table 3-11, as the REBUS-PC input is effectively identical, thereby demonstrating that the free format input and fixed format input are handled identically in REBUS-PC.

In verification test #14, the “overlay” option for geometry specification is tested, which is a key feature of the REBUS-PC code. In this test, the type 06 cards in the dataset A.NIP3 were modified such that each water channel covers the adjacent fuel plate in the outward R direction. In the verification test input, these cards are provided before the fuel plate cards, and thus REBUS-PC will overlay the fuel on the extra water regions when it encounters the fuel plate card inputs. An excerpt of the modified type 06 cards of A.NIP3 are shown in Figure 3-24, which should match the verification test #12 input provided in Figure 3-23. The modified portions are highlighted in Figure 3-24. The lines that “overlay” these inputs are also provided in Figure 3-24. If the “overlay” feature works as intended, the resulting model will be identical to the base model as the changes in Figure 3-24 only alter part

of the geometry that is redefined later. The results of verification test #14 are identical to those of verification tests #12 and #13 in Table 3-11, demonstrating that the overlay input feature is working properly.

Verification Test #12									
** water channels and fuel plates									
06	CL11E	0.00000E+00	7.85398E-01	0	5	6.72940E+00	8.45710E+00		
06	CL11F	0.00000E+00	7.85398E-01	5	10	6.72940E+00	8.45710E+00		
06	CL11G	0.00000E+00	7.85398E-01	10	15	6.72940E+00	8.45710E+00		
06	CL12E	0.00000E+00	7.85398E-01	0	5	9.71768E+00	1.14454E+01		
06	CL12F	0.00000E+00	7.85398E-01	5	10	9.71768E+00	1.14454E+01		
06	CL12G	0.00000E+00	7.85398E-01	10	15	9.71768E+00	1.14454E+01		
06	CL13E	0.00000E+00	7.85398E-01	0	5	1.27060E+01	1.44337E+01		
06	CL13F	0.00000E+00	7.85398E-01	5	10	1.27060E+01	1.44337E+01		
06	CL13G	0.00000E+00	7.85398E-01	10	15	1.27060E+01	1.44337E+01		
Verification Test #13									
** water channels and fuel plates									
06	CL11E	0.00000E+00	7.85398E-01	0	5	6.72940E+00	8.45710E+00		
06	CL11F	0.00000E+00	7.85398E-01	5	10	6.72940E+00	8.45710E+00		
06	CL11G	0.00000E+00	7.85398E-01	10	15	6.72940E+00	8.45710E+00		
06	CL12E	0.00000E+00	7.85398E-01	0	5	9.71768E+00	1.14454E+01		
06	CL12F	0.00000E+00	7.85398E-01	5	10	9.71768E+00	1.14454E+01		
06	CL12G	0.00000E+00	7.85398E-01	10	15	9.71768E+00	1.14454E+01		
06	CL13E	0.00000E+00	7.85398E-01	0	5	1.27060E+01	1.44337E+01		
06	CL13F	0.00000E+00	7.85398E-01	5	10	1.27060E+01	1.44337E+01		
06	CL13G	0.00000E+00	7.85398E-01	10	15	1.27060E+01	1.44337E+01		

Figure 3-23. Modified Geometry Inputs between Verification Tests #12 and #13

Verification Test #14									
** water channels and fuel plates									
06	CL11E	0.00000E+00	7.85398E-01	0	5	6.72940E+00	9.71768E+00		
06	CL11F	0.00000E+00	7.85398E-01	5	10	6.72940E+00	9.71768E+00		
06	CL11G	0.00000E+00	7.85398E-01	10	15	6.72940E+00	9.71768E+00		
06	CL12E	0.00000E+00	7.85398E-01	0	5	9.71768E+00	1.27060E+01		
06	CL12F	0.00000E+00	7.85398E-01	5	10	9.71768E+00	1.27060E+01		
06	CL12G	0.00000E+00	7.85398E-01	10	15	9.71768E+00	1.27060E+01		
06	CL13E	0.00000E+00	7.85398E-01	0	5	1.27060E+01	1.56942E+01		
06	CL13F	0.00000E+00	7.85398E-01	5	10	1.27060E+01	1.56942E+01		
06	CL13G	0.00000E+00	7.85398E-01	10	15	1.27060E+01	1.56942E+01		
Overlay Input that Un-does the Above Alterations									
06	FL11E	0.00000E+00	7.85398E-01	0	5	8.45710E+00	9.71768E+00		
06	FL11F	0.00000E+00	7.85398E-01	5	10	8.45710E+00	9.71768E+00		
06	FL11G	0.00000E+00	7.85398E-01	10	15	8.45710E+00	9.71768E+00		
06	FL12E	0.00000E+00	7.85398E-01	0	5	1.14454E+01	1.27060E+01		
06	FL12F	0.00000E+00	7.85398E-01	5	10	1.14454E+01	1.27060E+01		
06	FL12G	0.00000E+00	7.85398E-01	10	15	1.14454E+01	1.27060E+01		
06	FL13E	0.00000E+00	7.85398E-01	0	5	1.44337E+01	1.56942E+01		
06	FL13F	0.00000E+00	7.85398E-01	5	10	1.44337E+01	1.56942E+01		
06	FL13G	0.00000E+00	7.85398E-01	10	15	1.44337E+01	1.56942E+01		

Figure 3-24. Modified Geometry Inputs between Verification Tests #12 and #14

In addition to the input checking, the STRZ benchmark is used to check “color set” based cross section capabilities. A “color set” means that a different specific pre-processed set of multi-group cross sections are applied to different regions in the domain. In this regard, the test consists of verifying that by using different isotope labels, the mechanism to allow color sets in REBUS-PC, the correct cross section data is used in the specified spatial region. Because the mechanism to map zones to regions has already been checked, this is only the verification of the correct isotope usage in a given zone.

Figure 3-25 shows an excerpt of the color set input for REBUS-PC in the STRZ benchmark, where each fuel plate material defined in the geometry is assigned a specific set of isotopes. In order to complete the input setup, the depletion chain must be linked to each of these isotopes, as seen in the A.BURN section of input in the figure. To demonstrate that the regions have different cross sections, the ISOTXS binary file was setup to contain different cross sections for each of these isotopes as shown in Figure 3-26 for two example U-235 isotopes.

```

DATASET=A.NIP3
...
Material definitions used to define zones
13      MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 AL7A_0 3.2563E-02
13      MEAT1 U34A_0 1.0000E-20 U36A_0 1.0000E-20 SInA_0 7.5239E-03
13      MEAT1 NP7A_0 1.0000E-20 PU8A_0 1.0000E-20 PU9A_0 1.0000E-20
13      MEAT1 PU0A_0 1.0000E-20 PU1A_0 1.0000E-20 PU2A_0 1.0000E-20
13      MEAT1 AM1A_0 1.0000E-20 I35A_0 1.0000E-20 XE5A_0 1.0000E-20
13      MEAT1 PM9A_0 1.0000E-20 SM9A_0 1.0000E-20 LFPA_0 1.0000E-20
13      MEAT1 O16A_0 1.0000E-20
13      MEAT2 U35A_1 2.2518E-03 U38A_1 9.0341E-03 AL7A_1 3.2563E-02
13      MEAT2 U34A_1 1.0000E-20 U36A_1 1.0000E-20 SInA_1 7.5239E-03
13      MEAT2 NP7A_1 1.0000E-20 PU8A_1 1.0000E-20 PU9A_1 1.0000E-20
13      MEAT2 PU0A_1 1.0000E-20 PU1A_1 1.0000E-20 PU2A_1 1.0000E-20
13      MEAT2 AM1A_1 1.0000E-20 I35A_1 1.0000E-20 XE5A_1 1.0000E-20
13      MEAT2 PM9A_1 1.0000E-20 SM9A_1 1.0000E-20 LFPA_1 1.0000E-20
13      MEAT2 O16A_1 1.0000E-20
...
Zone definitions used in the depletion
14      FUEL1 MEAT1 3.9534E-01 AL-A 6.0466E-01
14      FUEL2 MEAT2 3.9534E-01 AL-A 6.0466E-01
...
DATASET=A.BURN
...
Isotope mapping for the depletion chain
10      I135 I35A_0I35C_0I35A_1I35A_2I35A_3
10      XE135 XE5A_0XE5C_0XE5A_1XE5A_2XE5A_3
10      PM149 PM9A_0PM9C_0PM9A_1PM9A_2PM9A_3
10      SM149 SM9A_0SM9C_0SM9A_1SM9A_2SM9A_3
10      U234 U34A_0U34C_0U34A_1U34A_2U34A_3
10      U235 U35A_0U35C_0U35A_1U35A_2U35A_3
...

```

Figure 3-25. Color Set Input Excerpt for Verification Test #12

The use of a particular isotope set in each zone will cause the homogenized cross sections in each zone to be unique and thus different cross sections will appear in those region. The first step in checking the input is to verify that the stated compositions consist of the correct isotopes and are assigned to the proper regions. The input for every zone was checked by manually comparing the atom density reported by REBUS-PC with the input provided in A.NIP3 via Excel. Table 3-12 shows a small selection of this comparison from the verification test #12 input and output.

The zone definitions are defined by card type 14 and are typically composed of different materials or even zones. Excel is again used to compute the final densities of every zone in the domain, but only a selection of the comparison is shown between the REBUS-PC computed values and the Excel calculation in Table 3-13. In both Table 3-12 and Table 3-13 one can see that the Excel calculation identically matches the REBUS-PC reported values. These results demonstrate that REBUS-PC correctly processes the material specifications on the type 13 cards and the composition specifications on the type 14 cards of A.NIP3.

```

[ISOTXS]...FILEWIDE ISOTOPE LABEL.....U35A_0
[ISOTXS]...GRAM ATOMIC WEIGHT.....0.235044006E+03
[ISOTXS]...TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS).....0.310375996E-10
[ISOTXS]...TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/CAPT).....0.104865997E-11
[ISOTXS]...GROUP    TRANS(P1)    TOTAL (P0)    (N,GAMMA)    FISSION    YIELD/FISS    CHI    .....
[ISOTXS]...    1    4.758010E+00    7.415620E+00    6.037540E-02    1.243730E+00    2.708840E+00    0.000000E+00    .....
[ISOTXS]...    2    9.689330E+00    1.120390E+01    4.318220E-01    1.652670E+00    2.447480E+00    0.000000E+00    .....
[ISOTXS]...    3    4.926690E+01    4.775680E+01    1.399940E+01    2.203170E+01    2.433800E+00    0.000000E+00    .....
[ISOTXS]...    4    5.868470E+01    5.878120E+01    9.703000E+00    3.643360E+01    2.435830E+00    0.000000E+00    .....
[ISOTXS]...    5    1.630000E+02    1.630850E+02    2.367730E+01    1.255160E+02    2.436700E+00    0.000000E+00    .....
[ISOTXS]...    6    3.001830E+02    3.002710E+02    4.215500E+01    2.438500E+02    2.436700E+00    0.000000E+00    .....
[ISOTXS]...    7    6.385090E+02    6.386070E+02    9.097700E+01    5.335290E+02    2.436700E+00    0.000000E+00    .....
...
[ISOTXS]...FILEWIDE ISOTOPE LABEL.....U35A_1
[ISOTXS]...GRAM ATOMIC WEIGHT.....0.235044006E+03
[ISOTXS]...TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS).....0.310375996E-10
[ISOTXS]...TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/CAPT).....0.104865997E-11
[ISOTXS]...GROUP    TRANS(P1)    TOTAL (P0)    (N,GAMMA)    FISSION    YIELD/FISS    CHI    .....
[ISOTXS]...    1    4.758050E+00    7.415630E+00    6.037670E-02    1.243730E+00    2.708830E+00    0.000000E+00    .....
[ISOTXS]...    2    9.690940E+00    1.120460E+01    4.319010E-01    1.652820E+00    2.447480E+00    0.000000E+00    .....
[ISOTXS]...    3    4.926520E+01    4.776500E+01    1.400310E+01    2.203630E+01    2.433800E+00    0.000000E+00    .....
[ISOTXS]...    4    5.868170E+01    5.877830E+01    9.703000E+00    3.643100E+01    2.435830E+00    0.000000E+00    .....
[ISOTXS]...    5    1.629430E+02    1.630290E+02    2.366480E+01    1.254730E+02    2.436700E+00    0.000000E+00    .....
[ISOTXS]...    6    2.988520E+02    2.989340E+02    4.201290E+01    2.426780E+02    2.436700E+00    0.000000E+00    .....
[ISOTXS]...    7    6.367970E+02    6.368930E+02    9.072650E+01    5.320970E+02    2.436700E+00    0.000000E+00    .....
...

```

Figure 3-26. ISOTXS Cross Sections Differences for Verification Test #12

Table 3-12. Manual Check of the Input Density for Card Type 13 in Verification Test #12

Material	Isotope Label	Density in Output	Density in Input	Diff.
MEAT1	AL7A_0	3.2563E-02	3.2563E-02	0.0000E+00
	AM1A_0	1.0000E-20	1.0000E-20	0.0000E+00
	I35A_0	1.0000E-20	1.0000E-20	0.0000E+00
	LFPA_0	1.0000E-20	1.0000E-20	0.0000E+00
	NP7A_0	1.0000E-20	1.0000E-20	0.0000E+00
	O16A_0	1.0000E-20	1.0000E-20	0.0000E+00
	PM9A_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU0A_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU1A_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU2A_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU8A_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU9A_0	1.0000E-20	1.0000E-20	0.0000E+00
	SInA_0	7.5239E-03	7.5239E-03	0.0000E+00
	SM9A_0	1.0000E-20	1.0000E-20	0.0000E+00
	U34A_0	1.0000E-20	1.0000E-20	0.0000E+00
	U35A_0	2.2518E-03	2.2518E-03	0.0000E+00
	U36A_0	1.0000E-20	1.0000E-20	0.0000E+00
	U38A_0	9.0341E-03	9.0341E-03	0.0000E+00
	XE5A_0	1.0000E-20	1.0000E-20	0.0000E+00
MEAT2	AL7C_0	3.2563E-02	3.2563E-02	0.0000E+00
	AM1C_0	1.0000E-20	1.0000E-20	0.0000E+00
	I35C_0	1.0000E-20	1.0000E-20	0.0000E+00
	LFPC_0	1.0000E-20	1.0000E-20	0.0000E+00
	NP7C_0	1.0000E-20	1.0000E-20	0.0000E+00
	O16C_0	1.0000E-20	1.0000E-20	0.0000E+00
	PM9C_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU0C_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU1C_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU2C_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU8C_0	1.0000E-20	1.0000E-20	0.0000E+00
	PU9C_0	1.0000E-20	1.0000E-20	0.0000E+00
	SInC_0	7.5239E-03	7.5239E-03	0.0000E+00
	SM9C_0	1.0000E-20	1.0000E-20	0.0000E+00
	U34C_0	1.0000E-20	1.0000E-20	0.0000E+00
	U35C_0	2.2518E-03	2.2518E-03	0.0000E+00
	U36C_0	1.0000E-20	1.0000E-20	0.0000E+00
	U38C_0	9.0341E-03	9.0341E-03	0.0000E+00
	XE5C_0	1.0000E-20	1.0000E-20	0.0000E+00

Table 3-13. Check of the Computed Densities for Card Type 14 in Verification Test #12

Composition	Isotope Label	REBUS-PC Reported Density	Calculated Density (Excel)	Diff.
FUEL1	AL7A_0	4.9312E-02	4.9312E-02	0.0000E+00
	AM1A_0	3.9534E-17	3.9534E-17	0.0000E+00
	I35A_0	3.9534E-17	3.9534E-17	0.0000E+00
	LFPA_0	3.9534E-17	3.9534E-17	0.0000E+00
	NP7A_0	3.9534E-17	3.9534E-17	0.0000E+00
	O16A_0	3.9534E-17	3.9534E-17	0.0000E+00
	PM9A_0	3.9534E-17	3.9534E-17	0.0000E+00
	PU0A_0	3.9534E-17	3.9534E-17	0.0000E+00
	PU1A_0	3.9534E-17	3.9534E-17	0.0000E+00
	PU2A_0	3.9534E-17	3.9534E-17	0.0000E+00
	PU8A_0	3.9534E-17	3.9534E-17	0.0000E+00
	PU9A_0	3.9534E-17	3.9534E-17	0.0000E+00
	SLnA_0	2.9745E-03	2.9745E-03	0.0000E+00
	SM9A_0	3.9534E-17	3.9534E-17	0.0000E+00
	U34A_0	3.9534E-17	3.9534E-17	0.0000E+00
	U35A_0	8.9023E-04	8.9023E-04	0.0000E+00
	U36A_0	3.9534E-17	3.9534E-17	0.0000E+00
	U38A_0	3.5715E-03	3.5715E-03	0.0000E+00
	XE5A_0	3.9534E-17	3.9534E-17	0.0000E+00
WCHNL	H01B_0	6.6691E-02	6.6691E-02	0.0000E+00
	O16B_0	3.3346E-02	3.3346E-02	0.0000E+00
CR_AL	AL7D_0	6.0263E-02	6.0263E-02	0.0000E+00
GRAPH	C12R_0	8.7240E-02	8.7240E-02	0.0000E+00
MIXXB	AL7B_0	4.4926E-02	4.4926E-02	0.0000E+00
	H01B_0	1.6973E-02	1.6973E-02	0.0000E+00
	O16B_0	8.4866E-03	8.4866E-03	0.0000E+00

In order to check whether the cross section data are referenced properly, the macroscopic cross sections of each composition must be compared. REBUS-PC can provide these details by turning on the fourth edit flag of the type 02 card of the dataset A.HMG4C. The homogenized cross sections were independently calculated using the MATLAB program [12] and the methodology for HMG4C described in the manual. For the STRZ benchmark, this produces a considerable amount of data. Consequently, only the comparison of the principal cross sections for one zone is shown in Table 3-14. As can be seen, there are minor differences observed between REBUS-PC and the Matlab calculation which are attributable to round off error in the computations of REBUS-PC.

To understand this, in REBUS-PC, the nuclide densities and macroscopic cross sections of each composition is stored in double precision (15 decimal place) containers, while the microscopic cross section data is stored in single precision (7 decimal place) containers. When carrying out floating point math, the resulting cross section data will at most have ~seven significant digit accuracy, and thus differences on the order of 10^{-7} are expected, as can be seen in Table 3-14.

Table 3-14. Macroscopic Principal Cross Sections of FUEL1 from Verification Test #12

	g	Total	Absorption	Removal	Transport	Fission	Nu*Fission	Chi	(n,2n)
MATLAB	1	3.098605E-03	1.872179E-01	2.165476E-02	1.172630E-01	2.509003E-03	6.908351E-03	7.654490E-01	7.404899E-05
	2	2.938379E-03	2.673692E-01	4.589980E-03	1.903871E-01	1.472945E-03	3.605147E-03	2.343930E-01	0.000000E+00
	3	5.941304E-02	2.229130E-01	6.007291E-02	2.118749E-01	1.961405E-02	4.773671E-02	1.602830E-04	0.000000E+00
	4	4.449686E-02	1.600869E-01	4.831203E-02	1.578015E-01	3.243417E-02	7.900412E-02	0.000000E+00	0.000000E+00
	5	1.384206E-01	2.552850E-01	1.472695E-01	2.529815E-01	1.117377E-01	2.722712E-01	0.000000E+00	0.000000E+00
	6	2.651013E-01	3.814249E-01	2.738767E-01	3.791968E-01	2.170818E-01	5.289632E-01	0.000000E+00	0.000000E+00
	7	5.760650E-01	6.903819E-01	5.840869E-01	6.880675E-01	4.749618E-01	1.157339E+00	0.000000E+00	0.000000E+00
REBUS-PC	1	3.098604E-03	1.872179E-01	2.165476E-02	1.172630E-01	2.509003E-03	6.908351E-03	7.654490E-01	7.404899E-05
	2	2.938378E-03	2.673692E-01	4.589979E-03	1.903871E-01	1.472944E-03	3.605147E-03	2.343930E-01	0.000000E+00
	3	5.941304E-02	2.229130E-01	6.007290E-02	2.118749E-01	1.961405E-02	4.773671E-02	1.602830E-04	0.000000E+00
	4	4.449686E-02	1.600869E-01	4.831203E-02	1.578014E-01	3.243417E-02	7.900412E-02	0.000000E+00	0.000000E+00
	5	1.384205E-01	2.552850E-01	1.472694E-01	2.529815E-01	1.117377E-01	2.722712E-01	0.000000E+00	0.000000E+00
	6	2.651013E-01	3.814249E-01	2.738767E-01	3.791968E-01	2.170818E-01	5.289632E-01	0.000000E+00	0.000000E+00
	7	5.760650E-01	6.903818E-01	5.840868E-01	6.880675E-01	4.749617E-01	1.157339E+00	0.000000E+00	0.000000E+00
Difference	1	3.23E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	2	3.40E-07	0.00E+00	2.18E-07	0.00E+00	6.79E-07	0.00E+00	0.00E+00	0.00E+00
	3	0.00E+00	0.00E+00	1.66E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	4	0.00E+00	0.00E+00	0.00E+00	6.34E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	5	7.22E-07	0.00E+00	6.79E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	7	0.00E+00	1.45E-07	1.71E-07	0.00E+00	2.11E-07	0.00E+00	0.00E+00	0.00E+00

To check whether the compositions were assigned to the correct spatial regions, i.e. card type 15 of A.NIP3, the assignment map of regions to composition zones was examined. The zone assignment output from REBUS-PC is tabulated in Table 3-15.

Table 3-15. REBUS-PC Zone Assignment to Region

Region No.	Region Name	Zone No.	Zone Name	Region No.	Region Name	Zone No.	Zone Name
1	UPSTR	10	ALBOX	131	FL12F	2	FUEL2
2	WPOOL	9	H2O	132	FL12G	2	FUEL2
3	FTRAP	8	FTH2O	133	FL13E	3	FUEL3
4	STWLI	3	MIXXB	134	FL13F	3	FUEL3
5	STWLO	5	MIXXD	135	FL13G	3	FUEL3
6	REFLT	7	GRAPH	136	FL14E	4	FUEL4
7	CL11E	2	WCHNL	137	FL14F	4	FUEL4
8	CL11F	2	WCHNL	138	FL14G	4	FUEL4
9	CL11G	2	WCHNL	223	BLDW1	10	CRH2O
10	CL12E	2	WCHNL	224	FOLL1	8	MIXXD
11	CL12F	2	WCHNL	225	BLAD1	7	FUELC
12	CL12G	2	WCHNL	226	HADL1	9	CR_AL
13	CL13E	2	WCHNL	227	BLDW2	10	CRH2O
14	CL13F	2	WCHNL	228	FOLL2	8	MIXXD
15	CL13G	2	WCHNL	229	BLAD2	7	FUELC
16	CL14E	2	WCHNL	230	HADL2	9	CR_AL
17	CL14F	2	WCHNL	231	BLDW3	10	CRH2O
18	CL14G	2	WCHNL	232	FOLL3	8	MIXXD
19	CL15E	2	WCHNL	233	BLAD3	7	FUELC
20	CL15F	2	WCHNL	234	HADL3	9	CR_AL
21	CL15G	2	WCHNL	235	BLDW4	10	CRH2O
127	FL11E	1	FUEL1	236	FOLL4	8	MIXXD
128	FL11F	1	FUEL1	237	BLAD4	7	FUELC
129	FL11G	1	FUEL1	238	HADL4	9	CR_AL
130	FL12E	2	FUEL2				

Due to the rotational symmetry of the STRZ model, only the fuel plate and water channel regions located in the first quadrant are shown. The reader should consult the input for verification test #12, an excerpt of which is provided in Figure 3-27, which shows that REBUS-PC zone to region information is fully consistent with the input.

Because verification test #13 is the free format input of verification test #12 (which used the fixed format of A.NIP3), and test #14 is effectively the same, the same comparisons as performed above result in no observable differences in the output. However, a detailed comparison of the output shows that verification test #13 and verification test #12 do differ on a few lines of the output. Of particular issue is the dominance ratio number, which is printed to 13 significant digits in the output and shows a difference in the 10th significant digit between the two tests. The different input processing performed by REBUS-PC for free format input versus fixed format leads to these slight differences in the floating point math. This magnitude of difference is not unusual for REBUS-PC.

15	MIXXB	STWLI			
15	FUELC	BLAD1	BLAD2	BLAD3	BLAD4
15	MIXXD	FOLL1	FOLL2	FOLL3	FOLL4
15	CR_AL	HADL1	HADL2	HADL3	HADL4
15	CRH2O	BLDW1	BLDW2	BLDW3	BLDW4
15	MIXXD	STWLO			
15	GRAPH	REFLT			
15	FTH2O	FTRAP			
15	H2O	WPOOL			
15	ALBOX	UPSTR			
15	FUEL1	FL11E	FL11F	FL11G	
15	FUEL2	FL12E	FL12F	FL12G	
15	FUEL3	FL13E	FL13F	FL13G	
15	FUEL4	FL14E	FL14F	FL14G	
15	FUEL1	FL21E	FL21F	FL21G	
15	FUEL2	FL22E	FL22F	FL22G	
15	FUEL3	FL23E	FL23F	FL23G	
15	FUEL4	FL24E	FL24F	FL24G	
...					

Figure 3-27. Zone to Region Assignment Input Excerpt for Verification Test #12

Capability 7 is focused on verifying the accuracy of the power edits for regions and areas. The processing of the A.NIP3 type 07 cards is first checked for area specifications against the REBUS-PC output, as illustrated in Figure 3-28. Given the previous verification of the region and area volumes, this check serves as a duplicative verification that REBUS-PC is processing the type 07 input correctly.

AREA NO. NAME	REGION NO. NAME	REGION NO. NAME	REGIONS COMPRISING AREAS					
			REGION NO. NAME	REGION NO. NAME	REGION NO. NAME	REGION NO. NAME	REGION NO. NAME	REGION NO. NAME
1 FUELX		127 FL11E	128 FL11F	129 FL11G	130 FL12E	131 FL12F	132 FL12G	133 FL13E
		134 FL13F	135 FL13G	136 FL14E	137 FL14F	138 FL14G	139 FL21E	140 FL21F
		141 FL21G	142 FL22E	143 FL22F	144 FL22G	145 FL23E	146 FL23F	147 FL23G
		148 FL24E	149 FL24F	150 FL24G	151 FL31E	152 FL31F	153 FL31G	154 FL32E
		155 FL32F	156 FL32G	157 FL33E	158 FL33F	159 FL33G	160 FL34E	161 FL34F
		162 FL34G	163 FL41E	164 FL41F	165 FL41G	166 FL42E	167 FL42F	168 FL42G
		169 FL43E	170 FL43F	171 FL43G	172 FL44E	173 FL44F	174 FL44G	175 FL51E
		176 FL51F	177 FL51G	178 FL52E	179 FL52F	180 FL52G	181 FL53E	182 FL53F
		183 FL53G	184 FL54E	185 FL54F	186 FL54G	187 FL61E	188 FL61F	189 FL61G
		190 FL62E	191 FL62F	192 FL62G	193 FL63E	194 FL63F	195 FL63G	196 FL64E
		197 FL64F	198 FL64G	199 FL71E	200 FL71F	201 FL71G	202 FL72E	203 FL72F
		204 FL72G	205 FL73E	206 FL73F	207 FL73G	208 FL74E	209 FL74F	210 FL74G
		211 FL81E	212 FL81F	213 FL81G	214 FL82E	215 FL82F	216 FL82G	217 FL83E
		218 FL83F	219 FL83G	220 FL84E	221 FL84F	222 FL84G		
		223 BLAD1	225 BLAD2	227 BLAD3	229 BLAD4			
	2 BLADE	127 FL11E	128 FL11F	129 FL11G	130 FL12E	131 FL12F	132 FL12G	133 FL13E
	3 BL&FL	134 FL13F	135 FL13G	136 FL14E	137 FL14F	138 FL14G	139 FL21E	140 FL21F
		141 FL21G	142 FL22E	143 FL22F	144 FL22G	145 FL23E	146 FL23F	147 FL23G
		148 FL24E	149 FL24F	150 FL24G	151 FL31E	152 FL31F	153 FL31G	154 FL32E
		155 FL32F	156 FL32G	157 FL33E	158 FL33F	159 FL33G	160 FL34E	161 FL34F
		162 FL34G	163 FL41E	164 FL41F	165 FL41G	166 FL42E	167 FL42F	168 FL42G
		169 FL43E	170 FL43F	171 FL43G	172 FL44E	173 FL44F	174 FL44G	175 FL51E
		176 FL51F	177 FL51G	178 FL52E	179 FL52F	180 FL52G	181 FL53E	182 FL53F
		183 FL53G	184 FL54E	185 FL54F	186 FL54G	187 FL61E	188 FL61F	189 FL61G
		190 FL62E	191 FL62F	192 FL62G	193 FL63E	194 FL63F	195 FL63G	196 FL64E
		197 FL64F	198 FL64G	199 FL71E	200 FL71F	201 FL71G	202 FL72E	203 FL72F

Figure 3-28. Excerpt of the Region to Area Assignment Edit for Verification Test #12

To check the power edits in the REBUS-PC output the region flux results provided by REBUS-PC and the power conversion factors printed in the macroscopic cross section edits are combined in Excel. Table 3-16 compares the region power edits in the REBUS-PC output with the values calculated using Excel. For brevity, only a small sample of regions is included, noting that all of the regions had similar accuracy. As can be seen, errors only appear in the sixth significant digit, as highlighted. These differences are traceable to round-off errors in the printed tables of region flux and power conversion factors.

Table 3-16. Region Power Comparison for Verification Test #12

Region No.	Region Name	Data from REBUS-PC Output			Excel
		Volume (cc)	Power Density (W/cc)	Region Power (W)	Region Power (W)
1	UPSTR	3.64817E+04	5.64615E-01	2.05981E+04	2.05981E+04
2	WPOOL	5.57556E+05	8.43067E-02	4.70057E+04	4.70057E+04
3	FTRAP	1.50000E+03	2.86018E+00	4.29025E+03	4.29025E+03
4	STWLI	2.76799E+03	3.37740E+00	9.34862E+03	9.34862E+03
5	STWLO	1.12490E+04	1.37837E+00	1.55053E+04	1.55053E+04
6	REFLT	2.24530E+04	2.05102E-02	4.60515E+02	4.60516E+02
7	CL11E	1.03035E+02	1.54423E+00	1.59110E+02	1.59110E+02
8	CL11F	1.03035E+02	1.29457E+00	1.33386E+02	1.33386E+02
9	CL11G	1.03035E+02	8.86429E-01	9.13335E+01	9.13334E+01
127	FL11E	8.99703E+01	9.58439E+02	8.62311E+04	8.62311E+04
128	FL11F	8.99703E+01	8.02991E+02	7.22454E+04	7.22454E+04
129	FL11G	8.99703E+01	5.58569E+02	5.02546E+04	5.02547E+04
223	BLAD1	1.40565E+03	3.67625E+02	5.16754E+05	5.16753E+05
224	HADL1	7.02826E+02	6.74158E-01	4.73816E+02	4.73815E+02

With the region power edits verified, it is a simple task to check the area edits. Table 3-17 shows the area powers extracted from the REBUS-PC output and the values calculated using Excel. Unlike the previous region power values, the area power values at three different time nodes were computed to further confirm the accuracy. As can be seen, the results are identical, thereby confirming the accuracy of the region and area power edits.

For completeness, the auxiliary table of burnup and power data produced by REBUS-PC in another output section is also checked. Table 3-18 provides the region power and burnup edits from REBUS-PC against those calculated using Excel. The burnup value was checked by using the initial mass of fissionable isotopes and the average daily fission power produced in each region as edited by REBUS-PC. From Table 3-18, one can see that the reported burnup edit and the Excel calculated values are consistent. The minor differences in the burnup values are again attributable to the limited precision of the edited values in the REBUS-PC output.

Table 3-17. Area Power Results for Verification Test #12

Time Node	Data Source	Area Powers (Watts)		
		FUELX	BLADE	BL&FL
0	Output Edit	7.81777E+06	2.06701E+06	9.88478E+06
	Excel	7.81777E+06	2.06701E+06	9.88478E+06
1	Output Edit	7.80138E+06	2.07915E+06	9.88053E+06
	Excel	7.80138E+06	2.07915E+06	9.88053E+06
10	Output Edit	7.84945E+06	2.02598E+06	9.87543E+06
	Excel	7.84945E+06	2.02598E+06	9.87543E+06

Table 3-18. Region FL11E Power and Burnup Edit Comparison for Verification Test #12

Time (Days)	Initial Mass of Fissionable Isotopes M_0 (Kg)	Average Daily Fission Power $\bar{P}_{fis}$ (MW)	REBUS-PC	Excel
			Ave. Burnup from Output (MWD/MT)	$\bar{P}_{fiss} \cdot \Delta T / M_0$ (MWD/MT) (ΔT - time interval)
0.0	1.58281E-01	0.00000E+00	0.00000E+00	0.00000E+00
3.0	1.58281E-01	8.48812E-02	1.60880E+03	1.60881E+03
6.0	1.58281E-01	8.43977E-02	1.59964E+03	1.59964E+03
9.0	1.58281E-01	8.42382E-02	1.59662E+03	1.59662E+03
12.0	1.58281E-01	8.41106E-02	1.59420E+03	1.59420E+03
15.0	1.58281E-01	8.39909E-02	1.59193E+03	1.59193E+03
18.0	1.58281E-01	8.38676E-02	1.58959E+03	1.58960E+03
21.0	1.58281E-01	8.37375E-02	1.58713E+03	1.58713E+03
24.0	1.58281E-01	8.36007E-02	1.58453E+03	1.58454E+03
27.0	1.58281E-01	8.34584E-02	1.58184E+03	1.58184E+03
30.0	1.58281E-01	8.33115E-02	1.57905E+03	1.57906E+03

Table 3-19 compares the instantaneous powers reported by REBUS-PC in the depletion section with the region powers edited in the flux solver module for region FL11E. It should be no surprise that the power results are consistent, indicating that the data is properly transferred from one section of the code to another.

Table 3-19. Region FL11E Instantaneous Power Comparison for Verification Test #12

Time (Days)	Region Instantaneous Power (MW)	Region Power Edited by DIF3D (MW)
0.0	8.62311E-02	8.62311E-02
3.0	8.56637E-02	8.56637E-02
6.0	8.54954E-02	8.54954E-02
9.0	8.53690E-02	8.53690E-02
12.0	8.52547E-02	8.52547E-02
15.0	8.51379E-02	8.51379E-02
18.0	8.50136E-02	8.50136E-02
21.0	8.48819E-02	8.48819E-02
24.0	8.47439E-02	8.47439E-02
27.0	8.46008E-02	8.46008E-02
30.0	8.44537E-02	8.44537E-02

The final capability to demonstrate with verification test #12 is the accuracy of the TYPE13.BCD files. The TYPE13.BCD file provide the zone atom density definitions and assignments to each region at each time node. Given that REBUS-PC only follows the fuel up to its discharge from the system, this capability is primarily used in complex shuffling schemes that are too difficult for REBUS-PC to handle directly. In these cases, the user intervenes and does intermediate decay and shuffling between different REBUS-PC loadings. Fundamentally, the output file provides users a means to construct a new, equivalent REBUS-PC input at each time point of a depletion cycle. The TYPE13.BCD file is

intentionally formatted for use in the A.NIP3 section of the REBUS-PC input. To verify the data in TYPE13.BCD is consistent with the REBUS-PC results is relatively easy, as REBUS-PC prints the same atom density information at the beginning of each time point. The comparison of the output shows that the TYPE13.BCD output is fully consistent with the REBUS-PC reported atom densities at each time point.

To verify its intended use, the TYPE13.BCD data was used to create a new REBUS-PC input file. If setup correctly, the resulting REBUS-PC calculation should identically reproduce the solution for the remainder of the depletion calculation of the originating REBUS-PC input. This modified input requires the material composition data (type 13, 14 and 15 cards of A.NIP3) to be replaced with those provided in TYPE13.BCD, in addition to modifications to the fuel management input card (type 35 card of A.BURN), such that it matches the original depletion steps from the chosen time node. Table 3-20 compares the k-effective results obtained from the original REBUS-PC calculation with that of the reconstructed input. Similarly, Table 3-21 compares the region-wise power of selected regions at the zeroth and fifth time nodes. One can see that the reconstructed input file using the TYPE13.BCD file produces nearly identical k-effective and region power results at each time node to the original input deck. The small errors are traceable to the input precision of the atom density information derived from TYPE13.BCD relative to data values stored internal to REBUS-PC.

Table 3-20. k-effective Results for First Step Reconstruction of Verification Test #12

Time Node	Time (day)	Original	Modified
0	0.0	1.097421 4	1.097421 5
1	3.0	1.049268 6	1.049268 7
2	6.0	1.043349 7	1.043349 8
3	9.0	1.038372 2	1.038372 3
4	12.0	1.034085 0	1.034085 1
5	15.0	1.0302067	1.0302067
6	18.0	1.026536 4	1.026536 5
7	21.0	1.0229592	1.0229592
8	24.0	1.019414 2	1.019414 3
9	27.0	1.015871 1	1.015871 2
10	30.0	1.012315 0	1.012315 1

An additional REBUS-PC input file was prepared using the material composition data and fuel management specifications from TYPE13.BCD at the seventh time node (21.0 days) of verification test #12. The k-effective results are compared in Table 3-22 and the region power data in Table 3-23 for each of the time nodes starting from 21.0 days. As was the case with the 0th time point, the k-effective and region powers show small errors with regards to the original input results at the same time points. These errors are again attributable to the input precision allowed by using the TYPE13.BCD data relative to the data stored internal to REBUS-PC.

Table 3-21. Power Results for First Step Reconstruction of Verification Test #12

Region Name	Region Power at BOC		Region Power after 15-day Irradiation	
	Original Input	Modified Input	Original Input	Modified Input
UPSTR	2.05981E+04	2.05981E+04	2.20371E+04	2.20371E+04
WPOOL	4.70057E+04	4.70057E+04	4.98223E+04	4.98223E+04
FTRAP	4.29025E+03	4.29025E+03	4.54431E+03	4.54431E+03
STWLI	9.34862E+03	9.34863E+03	9.87988E+03	9.87989E+03
STWLO	1.55053E+04	1.55053E+04	1.62998E+04	1.62998E+04
REFLT	4.60515E+02	4.60515E+02	4.83178E+02	4.83177E+02
CL11E	1.59110E+02	1.59110E+02	1.66818E+02	1.66818E+02
CL11F	1.33386E+02	1.33386E+02	1.40456E+02	1.40456E+02
CL11G	9.13335E+01	9.13334E+01	9.67413E+01	9.67413E+01
FL11E	8.62311E+04	8.62311E+04	8.51379E+04	8.51379E+04
FL11F	7.22454E+04	7.22454E+04	7.20151E+04	7.20151E+04
FL11G	5.02546E+04	5.02546E+04	5.08226E+04	5.08225E+04
BLAD1	5.16754E+05	5.16754E+05	5.14444E+05	5.14444E+05
HADL1	4.73816E+02	4.73816E+02	5.05679E+02	5.05679E+02

Table 3-22. k-effective Results for 7th Step Reconstruction of Verification Test #12

Time Node	Time (day)	Original	Modified
7	21.0	1.022959 ²	1.022959 ¹
8	24.0	1.019414 ²	1.019414 ¹
9	27.0	1.01587 ¹¹	1.01587 ⁰⁸
10	30.0	1.01231 ⁵⁰	1.01231 ⁴⁹

With the preceding results, verification tests #12 through #14 demonstrate the following capabilities:

- Capability 1, as it checks that the detailed input is processed correctly by REBUS-PC using all of the input pathways. In particular A.NIP3 card types 06, 07, 09, 13, 14, and 15 were thoroughly checked.
- Capability 2, as color set cross sections were defined and the homogenized cross sections were verified to be accurate within the floating point math being applied.
- Capability 3 is demonstrated, as all three of these verification use spatially dependent cross section data which leads to region dependent depletion behavior. However, the STRZ benchmark does not have a reference solution, and thus additional verification is required which is included later in this report.
- Capability 4 is additionally verified, as the reflected boundary condition is used.
- Capability 7 is demonstrated, as the region and area power integrals were checked using Excel.
- Capability 13 is demonstrated, as the TYPE13.BCD data was matched to the atom density output produced by REBUS-PC at each time point and was used to construct a new input that generated consistent results with the original input deck.

Table 3-23. Power Results for 7th Step Reconstruction of Verification Test #12

Region Name	Region Power after 21-day Irradiation		Region Power after 30-day Irradiation	
	Original Input	Modified Input	Original Input	Modified Input
UPSTR	2.22638E+04	2.22639E+04	2.26169E+04	2.26169E+04
WPOOL	5.01660E+04	5.01678E+04	5.06781E+04	5.06781E+04
FTRAP	4.58244E+03	4.58244E+03	4.63981E+03	4.63981E+03
STWLI	9.96571E+03	9.96573E+03	1.00954E+04	1.00954E+04
STWLO	1.64682E+04	1.64682E+04	1.67239E+04	1.67239E+04
REFLT	4.88776E+02	4.88774E+02	4.97272E+02	4.97272E+02
CL11E	1.68215E+02	1.68215E+02	1.70300E+02	1.70300E+02
CL11F	1.41772E+02	1.41772E+02	1.43775E+02	1.43775E+02
CL11G	9.77740E+01	9.77741E+01	9.93817E+01	9.93817E+01
FL11E	8.48819E+04	8.48820E+04	8.44537E+04	8.44537E+04
FL11F	7.20021E+04	7.20021E+04	7.19723E+04	7.19723E+04
FL11G	5.10221E+04	5.10222E+04	5.13486E+04	5.13486E+04
BLAD1	5.11371E+05	5.11369E+05	5.06496E+05	5.06496E+05
HADL1	5.10752E+02	5.10757E+02	5.18612E+02	5.18612E+02

3.11 Verification Test #15

Verification test #15 takes the STRZ geometry as its base input but is focused on satisfying capabilities #8 and #9. To do this, a zero (1 watt) power level is chosen along with a short depletion time and control rod movements. Because the previous verification test demonstrates that the flux solution capability of REBUS-PC is working, a new input geometry was constructed for each control rod position by manually inserting the meshes that are required and reassigning the materials, such that the expected (and observed) REBUS-PC input is reproduced at each time point. Using a low power prevents any change in the isotopic content and thereby demonstrates that REBUS-PC is correctly modifying the geometry and computing the correct solution at each time point.

The initial work focused on using two control rod banks, but a fatal error bug in the REBUS-PC software only allowed a single control rod bank to be used. Since the bug was not encountered before, it is obvious that all previous work using control rod movement was carried out using at most one control rod bank. Consequently, this verification test was tailored to have a single control rod bank with the specific inputs shown in Figure 3-29. To understand how this is done, the control rod tip position at each time point is provided, which can be identified by the region name FOLL1 from the input. A simple hump pattern of the control rod position is displayed in Figure 3-30.


```

DATASET=A.NIP3
...
06   BLDW1  0.00000E+00 1.57080E+00      0      1 2.31502E+01 2.44047E+01
06   FOLL1  0.00000E+00 1.57080E+00      1      2 2.31502E+01 2.44047E+01
06   BLAD1  0.00000E+00 1.57080E+00      2     15 2.31502E+01 2.44047E+01
06   HADL1  0.00000E+00 1.57080E+00     15     18 2.31502E+01 2.44047E+01
09   Z      5      10.0
09   Z      5      20.0
09   Z      5      30.0
09   Z      3      45.0
09   Z      2      50.0
09   Z      8      90.0
44   BANK1  FOLL1
...
DATASET=A.BURN
...
    *** time-dependent control rod positions
38   BANK1  0.00000E+00 2.0
38   BANK1  1.00000E+00 4.0
38   BANK1  2.00000E+00 6.0
38   BANK1  3.00000E+00 8.0
38   BANK1  4.00000E+00 6.0
38   BANK1  5.00000E+00 4.0
38   BANK1  6.00000E+00 2.0
...

```

Figure 3-29. Control Rod Input Details for Verification Test #15

Figure 3-30. Control Rod Tip Position for Verification Test #15

With regard to checking the output, the isotopic content is first verified to not change by extracting the total reactor loading at each time point. This data is plotted in Figure 3-31 and excerpts from time points 1 and 2 are shown in Figure 3-32. Note that only the U-235 and U-238 content are in the kg range and thus are plotted using the right hand scale, while the remaining isotopes are plotted using the left hand scale. From the output excerpt and compiled results, one can see that the total isotopic change over the 6 day depletion is minimal.

Figure 3-31. Isotope Reactor Loading (kg) for Verification Test #15

TOTAL REACTOR LOADING (IN KG) OF ACTIVE ISOTOPES AT TIME NODE 0 AT 0.00000E+00 DAYS.		TOTAL REACTOR LOADING (IN KG) OF ACTIVE ISOTOPES AT TIME NODE 1 AT 1.00000E+00 DAYS.	
ISOTOPE	REACTOR LOADING	ISOTOPE	REACTOR LOADING
I135	0.00000E+00	I135	1.39185E-11
XE135	0.00000E+00	XE135	1.38733E-11
PM149	0.00000E+00	PM149	6.26869E-12
SM149	0.00000E+00	SM149	1.03343E-12
U234	0.00000E+00	U234	7.30339E-14
U235	5.08129E+00	U235	5.08129E+00
U236	0.00000E+00	U236	2.20182E-10
U238	2.06467E+01	U238	2.06467E+01
NP237	0.00000E+00	NP237	3.59513E-13
PU238	0.00000E+00	PU238	2.59139E-23
PU239	0.00000E+00	PU239	1.33276E-10
PU240	0.00000E+00	PU240	1.50300E-20
PU241	0.00000E+00	PU241	4.53488E-30
PU242	0.00000E+00	PU242	2.03537E-40
AM241	0.00000E+00	AM241	1.49478E-34
LUMP	0.00000E+00	LUMP	5.41731E-10
DUMP	2.64406E+00	DUMP	2.64406E+00

Figure 3-32. Reactor Loading Output Excerpt for Verification Test #15

The next check is to verify that REBUS-PC correctly moves the control rod tip. From the input excerpt in Figure 3-29, and the tip position shown in Figure 3-30, the initial input specification defines the control rod tip at 2 cm. To verify this in the REBUS-PC input, the same checking mechanism shown earlier is used for verification tests #12 through #14, where the region map is checked with the region id list. Figure 3-33 shows the type of output that was used at each time point to identify the axial positions of each region in the control rod. To begin, the assigned region number for the control rod tip was identified at each time point. From there, the same region index was found in the region map output which gives the planes that the region fills. Finally, the axial meshing specifies the physical location of each plane.

	REGION NO.	REGION NAME	REGION VOLUME	ZONE NO.	ZONE NAME	ZONE CLASS.	BUCKLING BY GROUP (...)															
	221	FL84F	1.787E+02	4	FUEL4	0	0.000E+00															
	222	FL84G	1.787E+02	4	FUEL4	0	0.000E+00															
	223	BLDW1	9.371E+01	10	CRH2O	0	0.000E+00															
	224	FOLL1	9.371E+01	8	MIXXD	0	0.000E+00															
	225	BLAD1	1.218E+03	7	FUELC	0	0.000E+00															
	226	HADL1	7.028E+02	9	CR_AL	0	0.000E+00															
...																						
0	REACTOR REGION BY MESH POINT										Z	-DIM	MAP FOR PLANES				1	-	1			
	29	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6		

	28	*	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	*227	227		
	27	*	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	223	*227	227		

...																						
0	REACTOR REGION BY MESH POINT										Z	-DIM	MAP FOR PLANES				2	-	2			
...																						
	29	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6		

	28	*	224	224	224	224	224	224	224	224	224	224	224	224	224	224	224	224	*227	227		
	27	*	224	224	224	224	224	224	224	224	224	224	224	224	224	224	224	224	*227	227		

...																						
0	REACTOR REGION BY MESH POINT										Z	-DIM	MAP FOR PLANES				3	-	3			
	29	*	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6		

	28	*	225	225	225	225	225	225	225	225	225	225	225	225	225	225	225	225	*228	228		
	27	*	225	225	225	225	225	225	225	225	225	225	225	225	225	225	225	225	*228	228		

...																						
	Z- DIRECTION MESH INTERVAL BOUNDARIES																					
	1	0.00000E+00	2	2.00000E+00	3	4.00000E+00	4	6.00000E+00	5	8.00000E+00	6	1.00000E+01	7	1.20000E+01								
	8	1.40000E+01	9	1.60000E+01	10	1.80000E+01	11	2.00000E+01	12	2.20000E+01	13	2.40000E+01	14	2.60000E+01								
	15	2.80000E+01	16	3.00000E+01	17	3.50000E+01	18	4.00000E+01	19	4.50000E+01	20	4.75000E+01	21	5.00000E+01								
	22	5.50000E+01	23	6.00000E+01	24	6.50000E+01	25	7.00000E+01	26	7.50000E+01	27	8.00000E+01	28	8.50000E+01								
	29	9.00000E+01																				
...																						

Figure 3-33. REBUS-PC Output Excerpt Showing Control Rod Position Identification for Verification Test #15

Table 3-24 summarizes this effort for all time points, which verifies that the input provided to REBUS-PC is being correctly followed at each time point. It is important to note that the mesh boundaries of Table 3-24 are not present in Figure 3-29 such that REBUS-PC must introduce many of the meshes in order to construct the problem.

Table 3-24. Control Rod Material Location Identification for Verification Test #15.

Time Node (day)	Bank Position (cm)	Rod-tip Region Label	Mesh Cell in Channel	Lower Boundary of Regions in Control-rod Channel (cm)				
				BLDW1	FOLL1	BLAD1	HADL1	WPOOL
0.0	2.0	FOLL1	36	0.0	2.0	4.0	30.0	45.0
1.0	2.6	FOLL1	36	0.0	4.0	6.0	32.0	47.0
2.0	3.2	FOLL1	36	0.0	6.0	8.0	34.0	49.0
3.0	3.8	FOLL1	36	0.0	8.0	10.0	36.0	51.0
4.0	4.4	FOLL1	36	0.0	6.0	8.0	34.0	49.0
5.0	5.0	FOLL1	36	0.0	4.0	6.0	32.0	47.0
6.0	4.4	FOLL1	36	0.0	2.0	4.0	30.0	45.0

As discussed, the input was verified to construct new input geometries identical to the ones that result after the control rod movement and REBUS-PC produced the same results as that obtained at each time point. Table 3-25 provides the compiled REBUS-PC executable results for each time step. As can be seen, the results are identical to seven significant digits. Because the convergence criteria was set to 10^{-7} , there are notable minor differences in the results beyond the precision shown due to different initializations of the two calculations.

Table 3-25. Core Multiplication Factors at Each Time Node for Verification Test #15

Days	Control Rod Movement	Manually Created Equivalent Input
0	1.07899 592	1.07899 596
1	1.07879 025	1.07879 031
2	1.07596 887	1.07596 894
3	1.07383 873	1.07383 881
4	1.07596 887	1.07596 896
5	1.07879 024	1.07879 031
6	1.07899 588	1.07899 594

Because the composition does not change and the control rod positioning results in several time points with identical control rod positions (i.e., 0 and 6 days, 1 and 5 days, 2 and 4 days), one can see in Table 3-25 that these time points have the same multiplication factor.

The last part of this test to verify is that the flux and power output tables are identical between the control rod movement and the reproduced cases. As was the case from the previous STRZ verification tests, this is a vast amount of output detail and only an excerpt of that output is provided here as shown in Table 3-26. Time node 3 was selected and highlights the differences between the verification test and the manufactured comparison problems. As can be seen, the results shown are nearly identical and well within the input error tolerance of 10^{-5} . This output was taken from the

region and area power integral tables, an excerpt of which is shown in Figure 3-34, and which shows identical values to those that appear in Table 3-26.

Table 3-26. Time Node 3 Flux and Power Comparison for Verification Test #15

Region Name	Total Flux		Total Power		Group 4 Flux	
	Control Rod Movement	Manually Created	Control Rod Movement	Manually Created	Control Rod Movement	Manually Created
UPSTR	3.88388E+11	3.88389E+11	2.25499E-03	2.25499E-03	1.06079E+10	1.06079E+10
WPOOL	9.14268E+11	9.14269E+11	4.72191E-03	4.72191E-03	1.91490E+10	1.91490E+10
FTRAP	1.07838E+11	1.07838E+11	4.54780E-04	4.54780E-04	3.32989E+09	3.32989E+09
STWLI	1.73742E+11	1.73742E+11	9.90384E-04	9.90384E-04	6.34908E+09	6.34908E+09
STWLO	4.14279E+11	4.14279E+11	1.76088E-03	1.76088E-03	1.62570E+10	1.62570E+10
REFLT	5.55333E+11	5.55333E+11	5.52023E-05	5.52023E-05	2.06251E+10	2.06251E+10
CL11E	7.24628E+09	7.24628E+09	1.63942E-05	1.63942E-05	2.90022E+08	2.90022E+08
CL11F	6.21672E+09	6.21672E+09	1.40338E-05	1.40338E-05	2.48817E+08	2.48817E+08
CL11G	4.18432E+09	4.18432E+09	9.84139E-06	9.84139E-06	1.65013E+08	1.65013E+08
CL12E	8.76684E+09	8.76684E+09	1.16207E-05	1.16207E-05	3.93203E+08	3.93203E+08
CL12F	7.57513E+09	7.57513E+09	1.00273E-05	1.00273E-05	3.39668E+08	3.39668E+08
CL12G	5.09519E+09	5.09519E+09	7.13191E-06	7.13191E-06	2.26915E+08	2.26915E+08
CL13E	1.03926E+10	1.03926E+10	1.28822E-05	1.28822E-05	4.71056E+08	4.71056E+08
CL13F	9.07721E+09	9.07720E+09	1.12319E-05	1.12319E-05	4.11650E+08	4.11650E+08
CL13G	6.14520E+09	6.14520E+09	8.05979E-06	8.05979E-06	2.77210E+08	2.77210E+08
CL14E	1.12208E+10	1.12208E+10	1.50617E-05	1.50617E-05	5.02808E+08	5.02807E+08
CL14F	9.96205E+09	9.96205E+09	1.31524E-05	1.31524E-05	4.48995E+08	4.48995E+08
CL14G	6.81045E+09	6.81045E+09	9.46271E-06	9.46271E-06	3.05640E+08	3.05640E+08
CL15E	1.25135E+10	1.25135E+10	2.96187E-05	2.96187E-05	4.97513E+08	4.97513E+08
CL15F	1.11116E+10	1.11116E+10	2.36456E-05	2.36456E-05	4.62237E+08	4.62237E+08
CL15G	7.66313E+09	7.66313E+09	1.65601E-05	1.65601E-05	3.18132E+08	3.18132E+08
CL21E	7.24632E+09	7.24632E+09	1.63943E-05	1.63943E-05	2.90023E+08	2.90023E+08
CL21F	6.21675E+09	6.21675E+09	1.40339E-05	1.40339E-05	2.48818E+08	2.48818E+08
CL21G	4.18435E+09	4.18435E+09	9.84144E-06	9.84144E-06	1.65014E+08	1.65014E+08
CL22E	8.76688E+09	8.76688E+09	1.16208E-05	1.16208E-05	3.93205E+08	3.93205E+08
CL22F	7.57517E+09	7.57517E+09	1.00274E-05	1.00274E-05	3.39669E+08	3.39669E+08
CL22G	5.09522E+09	5.09522E+09	7.13195E-06	7.13195E-06	2.26916E+08	2.26916E+08
CL23E	1.03927E+10	1.03927E+10	1.28823E-05	1.28823E-05	4.71058E+08	4.71058E+08
CL23F	9.07725E+09	9.07725E+09	1.12319E-05	1.12319E-05	4.11652E+08	4.11652E+08
CL23G	6.14523E+09	6.14523E+09	8.05983E-06	8.05983E-06	2.77211E+08	2.77211E+08

In addition to these tables, the mesh wise flux and power tables were also compared, showing similar small differences. Based upon this work, the modeling of a single control rod bank is demonstrated to be correctly handled with REBUS-PC during fuel cycle operations.

0	REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(1.000E-05,1.000E+07)									
	REGION	ZONE	ZONE	VOLUME	INTEGRATION(1)	POWER	POWER DENSITY	PEAK DENSITY	PEAK TO AVG.	POWER
	NO.	NAME	NO.	NAME	(CC)	WEIGHT FACTOR	(WATTS)	(WATTS/CC)	(WATTS/CC) (2)	FRACTION
	1	UPSTR	1	UPSTR	3.64817E+04	1.00000E+00	2.25499E-03	6.18117E-08	2.10509E-07	3.40564E+00
	2	WPOOL	2	WPOOL	5.57275E+05	1.00000E+00	4.72191E-03	8.47321E-09	1.26680E-07	1.49506E+01
	3	FTRAP	3	FTRAP	1.50000E+03	1.00000E+00	4.54780E-04	3.03188E-07	4.29554E-07	1.41679E+00
	4	STWLI	4	STWLI	2.76799E+03	1.00000E+00	9.90384E-04	3.57799E-07	5.03574E-07	1.40742E+00
	5	STWLO	5	STWLO	1.12490E+04	1.00000E+00	1.76088E-03	1.56537E-07	2.52705E-07	1.61435E+00
	6	REFLT	6	REFLT	2.24530E+04	1.00000E+00	5.52023E-05	2.45857E-09	4.35714E-09	1.77222E+00
	7	CL11E	7	CL11E	1.03035E+02	1.00000E+00	1.63942E-05	1.59112E-07	2.18176E-07	1.37121E+00
	8	CL11F	8	CL11F	1.03035E+02	1.00000E+00	1.40338E-05	1.36204E-07	1.99644E-07	1.46578E+00
	9	CL11G	9	CL11G	1.03035E+02	1.00000E+00	9.84139E-06	9.55148E-08	1.50663E-07	1.57737E+00
	10	CL12E	10	CL12E	1.43586E+02	1.00000E+00	1.16207E-05	8.09323E-08	8.71538E-08	1.07687E+00
	11	CL12F	11	CL12F	1.43586E+02	1.00000E+00	1.00273E-05	6.98348E-08	8.13928E-08	1.16550E+00
	12	CL12G	12	CL12G	1.43586E+02	1.00000E+00	7.13191E-06	4.96700E-08	6.48331E-08	1.30528E+00
...										
	REGION	ZONE	ZONE	VOLUME	TOTAL FLUX	PEAK FLUX (1)	TOTAL FAST FLUX	PEAK FAST FLUX(1)		
	NO.	NAME	NO.	NAME	(CC)	(NEUTRON-CM/SEC)	(NEUTRON/CM2-SEC)	(NEUTRON-CM/SEC)	(NEUTRON/CM2-SEC)	
	1	UPSTR	1	UPSTR	3.64817E+04	3.88388E+11	3.48177E+07	5.66910E+10	9.00224E+06	
	2	WPOOL	2	WPOOL	5.57275E+05	9.14268E+11	2.82289E+07	9.21790E+10	4.74176E+06	
	3	FTRAP	3	FTRAP	1.50000E+03	1.07838E+11	9.55896E+07	1.71630E+10	1.69358E+07	
	4	STWLI	4	STWLI	2.76799E+03	1.73742E+11	8.13515E+07	4.02435E+10	2.04406E+07	
	5	STWLO	5	STWLO	1.12490E+04	4.14279E+11	5.31318E+07	1.08193E+11	1.40428E+07	
	6	REFLT	6	REFLT	2.24530E+04	5.55333E+11	3.89667E+07	1.24215E+11	1.07331E+07	
	7	CL11E	7	CL11E	1.03035E+02	7.24628E+09	7.80907E+07	2.19097E+09	2.43894E+07	
	8	CL11F	8	CL11F	1.03035E+02	6.21672E+09	7.15879E+07	1.88325E+09	2.24549E+07	
	9	CL11G	9	CL11G	1.03035E+02	4.18432E+09	5.49478E+07	1.23374E+09	1.69171E+07	
	10	CL12E	10	CL12E	1.43586E+02	8.76684E+09	6.35309E+07	3.41846E+09	2.50894E+07	
	11	CL12F	11	CL12F	1.43586E+02	7.57513E+09	5.93852E+07	2.95578E+09	2.31283E+07	
	12	CL12G	12	CL12G	1.43586E+02	5.09519E+09	4.60179E+07	1.95317E+09	1.77710E+07	
	13	CL13E	13	CL13E	1.84134E+02	1.03926E+10	5.91390E+07	4.13338E+09	2.44302E+07	
...										
0	REGION AND AREA REAL FLUX INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(1.000E-05,1.000E+07)0									
	REGION	ZONE	ZONE	GROUP	GROUP	GROUP	GROUP	GROUP	GROUP	GROUP
	NO.	NAME	NO.	NAME	1	2	3	4	5	6
	1	UPSTR	1	UPSTR	3.90786E+10	4.18306E+10	3.74495E+10	1.06079E+10	6.24295E+09	9.40803E+10
	2	WPOOL	2	WPOOL	6.30212E+10	6.92514E+10	6.61580E+10	1.91490E+10	1.17274E+10	2.51060E+11
	3	FTRAP	3	FTRAP	1.18575E+10	1.26007E+10	1.19264E+10	3.32989E+09	2.02810E+09	2.53883E+10
	4	STWLI	4	STWLI	2.75257E+10	3.02056E+10	2.50908E+10	6.34908E+09	3.95877E+09	3.55734E+10
	5	STWLO	5	STWLO	7.42989E+10	8.05012E+10	6.46431E+10	1.62570E+10	9.77779E+09	7.40829E+10
	6	REFLT	6	REFLT	8.17443E+10	1.00871E+11	8.04257E+10	2.06251E+10	1.19453E+10	1.11031E+11
	7	CL11E	7	CL11E	1.51193E+09	1.61274E+09	1.18656E+09	2.90022E+08	1.69328E+08	1.12854E+09
...										

Figure 3-34. REBUS-PC Output Excerpt Showing Core Power and Flux Data Compared for Verification Test #15

With the preceding work, verification test #15 demonstrates the following capabilities:

- Capability 8, as it verifies that the control rod movement is properly handled by REBUS-PC for a single control rod bank.
- Capability 9, as it verifies the remeshing required to handle new movement of fixed control rod boundaries is handled properly by REBUS-PC.

This verification test also provides addition demonstration of capabilities 1, 2, 3, 4, and 7, but provides no additional information than that previously derived from the STRZ verification tests #12 through #14.

3.12 Verification Tests #16 and #17

These verification tests are focused on addressing another part of capability 1. As part of capability 1, REBUS-PC must be verified to execute identically when provided the A.ISO and the binary file ISOTXS microscopic cross section input. Verification test #16 uses the A.ISO, an excerpt of which is provided in Figure 3-35. The input for this verification test is considerably longer than that of verification test #17, which uses the binary ISOTXS file. Both of these tests are exact duplicates of verification test #19 discussed later. In the case of verification test #17, modified comment cards are the only reason it produces a different output from verification test #19.

```

NOSORT=A.ISO
0V ISOTXS *CELLW WATER *      0
1D      7 1053      6      6      2      1      4      1
2D *iaea10 cella: U3SI2 19.75% 4.45 gU/cc 23/17plates *
*      * H01A_0 O16A_0 U35A_0 U36A_0 U34A_0 PU8A_0 PU9A_0 PU0A_0 PU1A_0
PU2A_0 AM1A_0 NP7A_0 XE5A_0 SM9A_0 I35A_0 PM9A_0 AL7A_0 U38A_0 SInA_0
LFPA_0 H01A_1 O16A_1 U35A_1 U36A_1 U34A_1 PU8A_1 PU9A_1 PU0A_1 PU1A_1
PU2A_1 AM1A_1 NP7A_1 XE5A_1 SM9A_1 I35A_1 PM9A_1 AL7A_1 U38A_1 SInA_1
LFPA_1 H01A_2 O16A_2 U35A_2 U36A_2 U34A_2 PU8A_2 PU9A_2 PU0A_2 PU1A_2
PU2A_2 AM1A_2 NP7A_2 XE5A_2 SM9A_2 I35A_2 PM9A_2 AL7A_2 U38A_2 SInA_2
LFPA_2 H01A_3 O16A_3 U35A_3 U36A_3 U34A_3 PU8A_3 PU9A_3 PU0A_3 PU1A_3
...
7.65449E-01 2.34393E-01 1.60283E-04 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00
1.96536E+09 3.85069E+08 1.15801E+07 1.68164E+06 8.68918E+05 4.51316E+05
2.23361E+05 1.00000E+07 8.21000E+05 5.53000E+03 4.00000E+00 6.25000E-01
2.50000E-01 5.80000E-02 1.00000E-05
      0      4      9      15      21      27      33      39      45      51      57      63
      69      74      80      85      90      95      101      107      113      117      122      128
...
4D H01A_0 (blan      20
1.00783E+00 0.00000E+00 3.56423E-13 2.96000E+02 2.04780E+01 4.22119E-02
      0      0      0      0      0      0      0      0      1      0      0
      100      200      300      2      2      0      0      7      7      7      7      7
      7      7      7      7      7      7      7      7      7      7      7
      7      7      7      7      7      7      7      7      7      7      7
      6      5      4      3      2      1      7      6      5      4      3      2
      1      7      6      5      4      3      2      1      7      6      5      4
      3      2      1
5D 1.76504E+00 3.94199E+00 6.90667E+00 8.73243E+00 1.30255E+01
2.23376E+01 4.18063E+01 2.93167E+00 1.11938E+01 2.03603E+01 2.13010E+01
2.48341E+01 3.42657E+01 5.38613E+01 3.46060E-05 1.49470E-04 6.63084E-03
4.39965E-02 8.53817E-02 1.66568E-01 3.41006E-01
...

```

Figure 3-35. REBUS-PC A.ISO Input Excerpt for Verification Test #16

The A.ISO file format is the ascii version of the data stored in the binary ISOTXS file. As expected, verification tests #16 and #17 produce identical answers within the small round off errors caused by the precision of the numbers in the ascii versus the binary versions of the cross section data, which

has a negligible impact on the answers. Because the output files are identical to verification test #19, all output excerpts are deferred to the discussion of verification test #19. Duplication of verification test #19 was chosen as its usage of the ISOTXS data (cross section interpolation) is the most complex of all of the test problems.

With the preceding analysis, these verification test demonstrate the following capability:

- Capability 2, as it verifies that the ASCII and binary ISOTXS input yield equivalent results

3.13 Verification Tests #18, #19, and #20

These verification tests are designed to verify capabilities 11 and 12. The way that this is accomplished is by reproducing the cross section interpolation for several regions and verifying it against the output of REBUS-PC. It is important to note that this action also supports capability #3 as it proves REBUS-PC is using specific ISOTXS cross sections in specific regions for the STRZ benchmark.

Figure 3-36 shows an excerpt of the A.BURN input for verification test #19 specifying burnup dependent cross sections of U-238. The type 26 cards specify the labels of the reference base isotope and the isotopes with burnup dependent cross sections. The type 39 cards specify the burnup dependent energy groups, and the type 40 cards specify the allowable error in the absolute value of the relative residue in the polynomial or spline fit. The type 41 cards specify the labels of isotopes in the ISOTXS library whose cross sections are included in the polynomial or spline fit and the corresponding number densities of the reference isotope.

BURNUP DEPENDENT XS DATA FOR U38A_0, DEPENDING ON U35A_0 NUMBER DENSITY									
26	U35A_0U38A_0								
39	U35A_0	1	7U38A_0	1	7PU9A_0	1	7		
39	U35C_0	1	7U38C_0	1	7PU9C_0	1	7		
39	LFP A_0	1	7LFPC_0	1	7				
40	U38A_0	31	1.0-3	8U38A_0	32	1.0-3	8		
41	U38A_0U38A_0	8.90249E-04	1.0+3	U38A_1	8.87191E-04		1.0		
41	U38A_0U38A_2	8.84131E-04	1.0	U38A_3	8.81076E-04		1.0		
41	U38A_0U38A_4	8.74968E-04	1.0	U38A_5	8.68874E-04		1.0		
41	U38A_0U38A_6	8.65830E-04	1.0	U38A_7	8.53699E-04		1.0		
41	U38A_0U38A_8	8.41609E-04	1.0	U38A_9	8.29566E-04		1.0		
41	U38A_0U38A10	8.23559E-04	1.0	U38A11	7.99701E-04		1.0		
41	U38A_0U38A12	7.76015E-04	1.0	U38A13	7.52494E-04		1.0		
41	U38A_0U38A14	7.40798E-04	1.0	U38A15	6.94709E-04		1.0		
41	U38A_0U38A16	6.49282E-04	1.0	U38A17	6.04544E-04		1.0		
41	U38A_0U38A18	5.82434E-04	1.0	U38A19	4.97058E-04		1.0		
41	U38A_0U38A20	4.14788E-04	1.0	U38A21	3.35994E-04		1.0		
41	U38A_0U38A22	2.98069E-04	1.0	U38A23	2.28978E-04		1.0		
41	U38A_0U38A24	1.65557E-04	1.0	U38A25	1.09277E-04		1.0		

Figure 3-36. REBUS-PC A.BURN Input Excerpt for Verification Test #19

During the execution of REBUS-PC, an auxiliary output file POLYFI.BCD is generated when the burnup dependent cross section option is invoked. Figure 3-37 and Figure 3-38 show the details of the POLYFI.BCD file which provides the input specification for burnup dependent cross section data and example interpolated relative cross section data at the mid-point of each atom density interval with respect to the reference isotope density (denoted by the column "X").

By comparing the input data specified on the type 41 cards of the A.BURN dataset with the input cross sections saved in the output file POLYFI.BCD, the burnup dependent cross section data can be verified. The interpolated cross sections of REBUS-PC were verified by comparing them with the reference values obtained with a MATLAB program. The MATLAB script to perform the cubic spline

interpolation of burnup dependent cross sections is provided in the repository. Figure 3-39 compares isotopic cross section data with the interpolated equivalent for the (n, γ) cross section of U-238 in the STRZ fuel composition. As can be seen, the two sets of cross sections appear identical and upon detailed inspection are accurate to the precision of the stored data.

INPUT CROSS SECTIONS FOR ISOTOPE U38A_0 GROUP 2							
X	CAPTURE	FISSION	N,P	N,ALPHA	N,D	N,T	
1	1.09277E-04	2.56253E-01	4.74041E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	1.65557E-04	2.56198E-01	4.74107E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	2.28978E-04	2.56169E-01	4.74118E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	2.98069E-04	2.56138E-01	4.74134E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	3.35994E-04	2.56120E-01	4.74147E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6	4.14788E-04	2.56133E-01	4.74083E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7	4.97058E-04	2.56109E-01	4.74085E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8	5.82434E-04	2.56088E-01	4.74084E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9	6.04544E-04	2.56036E-01	4.74163E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10	6.49282E-04	2.56019E-01	4.74171E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11	6.94709E-04	2.56003E-01	4.74178E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12	7.40798E-04	2.55983E-01	4.74194E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13	7.52494E-04	2.55978E-01	4.74195E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14	7.76015E-04	2.55970E-01	4.74199E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15	7.99701E-04	2.55962E-01	4.74202E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
16	8.23559E-04	2.55953E-01	4.74204E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
17	8.29566E-04	2.55951E-01	4.74204E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
18	8.41609E-04	2.55993E-01	4.74131E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
19	8.53699E-04	2.55989E-01	4.74132E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
20	8.65830E-04	2.55986E-01	4.74133E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
21	8.68874E-04	2.55985E-01	4.74133E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
22	8.74968E-04	2.55983E-01	4.74133E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
23	8.81076E-04	2.55982E-01	4.74134E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
24	8.84131E-04	2.55981E-01	4.74134E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
25	8.87191E-04	2.55980E-01	4.74135E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
26	8.90249E-04	2.55930E-01	4.74218E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

Figure 3-37. POLYFI.BCD Excerpt for a Cubic Spline Fit in Verification Test #19

INTERPOLATED RELATIVE CROSS SECTIONS FOR ISOTOPE U38A_0 GROUP 2							
X	CAPTURE	FISSION	N,P	N,ALPHA	N,D	N,T	
1	1.37417E-04	1.00114E+00	9.99707E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	1.97267E-04	1.00098E+00	9.99789E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	2.63523E-04	1.00088E+00	9.99797E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	3.17032E-04	1.00077E+00	9.99843E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	3.75391E-04	1.00076E+00	9.99788E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6	4.55923E-04	1.00074E+00	9.99724E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7	5.39746E-04	1.00075E+00	9.99630E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8	5.93489E-04	1.00051E+00	9.99804E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9	6.26913E-04	1.00034E+00	9.99930E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10	6.71996E-04	1.00033E+00	9.99896E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11	7.17754E-04	1.00024E+00	9.99937E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12	7.46646E-04	1.00020E+00	9.99951E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13	7.64254E-04	1.00017E+00	9.99955E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14	7.87858E-04	1.00014E+00	9.99966E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15	8.11630E-04	1.00012E+00	9.99960E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
16	8.26563E-04	1.00008E+00	9.99977E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
17	8.35588E-04	1.00016E+00	9.99898E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
18	8.47654E-04	1.00026E+00	9.99801E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
19	8.59765E-04	1.00022E+00	9.99824E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
20	8.67352E-04	1.00022E+00	9.99821E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
21	8.71921E-04	1.00021E+00	9.99821E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
22	8.78022E-04	1.00021E+00	9.99820E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
23	8.82603E-04	1.00020E+00	9.99826E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
24	8.85661E-04	1.00021E+00	9.99811E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
25	8.88720E-04	1.00012E+00	9.99895E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

Figure 3-38. POLYFI.BCD Interpolated Cross Section for Verification Test #19

Figure 3-39. Group Two (n, γ) Capture Cross Sections of U-238 for Verification Test #19

All of the isotopes specified as burnup dependent in REBUS-PC can be compared with the MATLAB program results for the same data. The interpolated cross sections of REBUS-PC and MATLAB were written to ASCII files with the same format as POLYFI.BCD. As an example, Figure 3-40 compares the burnup dependent cross sections for group 1 of the lumped fission product isotope LFPA_0. The upper section shows REBUS-PC result while the lower section shows the MATLAB program and the highlighting shows which lines differ and which parts of each line are different. A quick inspection of the output shows that the results only differ in the last significant digit, which is consistent with the accuracy of the math in REBUS-PC (single precision).

Given that the cubic spline fit of the cross section data is verified, its usage by REBUS-PC must be verified. This is easy to verify as REBUS-PC can print out the macroscopic cross sections used at each time node in each region or the microscopic cross sections and the atom densities of each region. Because the interpolation is based upon the calculated atom density, the atom density printout is combined with the macroscopic cross section print out for the verification. Figure 3-41 shows the output excerpt taken for the macroscopic cross section data, where previous excerpts have shown the typical atom density printout. MATLAB is again used to compute the macroscopic cross sections given the evaluation of the microscopic cross section using the spline fit. This involved the interpolation of numerous isotopic cross sections (U-235, U-238, Pu-239, LFP, Xe-135, etc...) given the density of the reference isotope (U-235). Because of the extensive amount of output that this generates, only a sample of the fission cross section comparison is provided in Figure 3-42 for region FL11E. The verification test has 11 distinct time node outputs and the information from Figure 3-41 is condensed from all 11 time nodes to create Figure 3-42.

As was the case with the microscopic cross section comparison, the differences between the REBUS-PC and MATLAB calculations only appear in the sixth significant digit, which is within the limits of the math precision. Similar errors were observed from additional comparisons for other regions and reactions. The results demonstrate that the cubic spline routine of REBUS-PC correctly performs the cross section interpolation consistent with that described in the manual and thus satisfies

capability 11. In addition, the isotopes specified in the ISOTXS file are properly linked to the region of interest, thereby demonstrating capability 3.

	X	CAPTURE	FISSION	N, P	N, ALPHA	N, D	N, T
1	1.37417E-04	1.76529E-02	0.00000E+00	2.29344E-05	1.80423E-05	2.64447E-08	2.57397E-09
2	1.97267E-04	1.81202E-02	0.00000E+00	2.35026E-05	1.89818E-05	2.57509E-08	2.56892E-09
3	2.63523E-04	1.85376E-02	0.00000E+00	2.40097E-05	1.97873E-05	2.51591E-08	2.56211E-09
4	3.17032E-04	1.87915E-02	0.00000E+00	2.43172E-05	2.03026E-05	2.46998E-08	2.55056E-09
5	3.75391E-04	1.89853E-02	0.00000E+00	2.45478E-05	2.07389E-05	2.41850E-08	2.53038E-09
6	4.55923E-04	1.92243E-02	0.00000E+00	2.48353E-05	2.12585E-05	2.35802E-08	2.50435E-09
7	5.39746E-04	1.94584E-02	0.00000E+00	2.51232E-05	2.17368E-05	2.30712E-08	2.48082E-09
8	5.93489E-04	1.95797E-02	0.00000E+00	2.52768E-05	2.19943E-05	2.27710E-08	2.46457E-09
9	6.26913E-04	1.96355E-02	0.00000E+00	2.53471E-05	2.21259E-05	2.25771E-08	2.45250E-09
10	6.71996E-04	1.97090E-02	0.00000E+00	2.54362E-05	2.22894E-05	2.23292E-08	2.43625E-09
11	7.17754E-04	1.97913E-02	0.00000E+00	2.55354E-05	2.24506E-05	2.21046E-08	2.42138E-09
12	7.46646E-04	1.98342E-02	0.00000E+00	2.55851E-05	2.25336E-05	2.19604E-08	2.41116E-09
13	7.64254E-04	1.98518E-02	0.00000E+00	2.56037E-05	2.25706E-05	2.18661E-08	2.40407E-09
14	7.87858E-04	1.98701E-02	0.00000E+00	2.56226E-05	2.26081E-05	2.17405E-08	2.39453E-09
15	8.11630E-04	1.98789E-02	0.00000E+00	2.56374E-05	2.26282E-05	2.16223E-08	2.38562E-09
16	8.26563E-04	1.98623E-02	0.00000E+00	2.56303E-05	2.26130E-05	2.15456E-08	2.37970E-09
17	8.35588E-04	1.98360E-02	0.00000E+00	2.56121E-05	2.25828E-05	2.14951E-08	2.37566E-09
18	8.47654E-04	1.97747E-02	0.00000E+00	2.55684E-05	2.25054E-05	2.14278E-08	2.37025E-09
19	8.59765E-04	1.96722E-02	0.00000E+00	2.54847E-05	2.23453E-05	2.13653E-08	2.36541E-09
20	8.67352E-04	1.95813E-02	0.00000E+00	2.53758E-05	2.21416E-05	2.13238E-08	2.36212E-09
21	8.71921E-04	1.95179E-02	0.00000E+00	2.52694E-05	2.19442E-05	2.12955E-08	2.35982E-09
22	8.78022E-04	1.94415E-02	0.00000E+00	2.50441E-05	2.15239E-05	2.12624E-08	2.35709E-09
23	8.82603E-04	1.94121E-02	0.00000E+00	2.47645E-05	2.09992E-05	2.12257E-08	2.35433E-09
24	8.85661E-04	1.94240E-02	0.00000E+00	2.44902E-05	2.04852E-05	2.12242E-08	2.35379E-09
25	8.88720E-04	1.94704E-02	0.00000E+00	2.41129E-05	1.97687E-05	2.11010E-08	2.34649E-09

	X	CAPTURE	FISSION	N, P	N, ALPHA	N, D	N, T
1	1.37417E-04	1.76529E-02	0.00000E+00	2.29344E-05	1.80423E-05	2.64447E-08	2.57398E-09
2	1.97267E-04	1.81202E-02	0.00000E+00	2.35026E-05	1.89818E-05	2.57510E-08	2.56892E-09
3	2.63523E-04	1.85376E-02	0.00000E+00	2.40098E-05	1.97873E-05	2.51591E-08	2.56211E-09
4	3.17032E-04	1.87915E-02	0.00000E+00	2.43171E-05	2.03026E-05	2.46997E-08	2.55056E-09
5	3.75391E-04	1.89853E-02	0.00000E+00	2.45479E-05	2.07390E-05	2.41850E-08	2.53037E-09
6	4.55923E-04	1.92243E-02	0.00000E+00	2.48352E-05	2.12584E-05	2.35802E-08	2.50435E-09
7	5.39746E-04	1.94584E-02	0.00000E+00	2.51233E-05	2.17368E-05	2.30713E-08	2.48082E-09
8	5.93489E-04	1.95798E-02	0.00000E+00	2.52769E-05	2.19944E-05	2.27710E-08	2.46457E-09
9	6.26913E-04	1.96355E-02	0.00000E+00	2.53470E-05	2.21258E-05	2.25772E-08	2.45249E-09
10	6.71996E-04	1.97089E-02	0.00000E+00	2.54361E-05	2.22894E-05	2.23291E-08	2.43625E-09
11	7.17754E-04	1.97913E-02	0.00000E+00	2.55354E-05	2.24506E-05	2.21046E-08	2.42137E-09
12	7.46646E-04	1.98342E-02	0.00000E+00	2.55850E-05	2.25335E-05	2.19604E-08	2.41116E-09
13	7.64254E-04	1.98519E-02	0.00000E+00	2.56037E-05	2.25705E-05	2.18660E-08	2.40408E-09
14	7.87858E-04	1.98701E-02	0.00000E+00	2.56227E-05	2.26081E-05	2.17406E-08	2.39453E-09
15	8.11630E-04	1.98789E-02	0.00000E+00	2.56374E-05	2.26282E-05	2.16222E-08	2.38562E-09
16	8.26563E-04	1.98623E-02	0.00000E+00	2.56302E-05	2.26129E-05	2.15455E-08	2.37970E-09
17	8.35588E-04	1.98359E-02	0.00000E+00	2.56121E-05	2.25828E-05	2.14950E-08	2.37565E-09
18	8.47654E-04	1.97748E-02	0.00000E+00	2.55685E-05	2.25053E-05	2.14277E-08	2.37025E-09
19	8.59765E-04	1.96722E-02	0.00000E+00	2.54847E-05	2.23454E-05	2.13652E-08	2.36541E-09
20	8.67352E-04	1.95812E-02	0.00000E+00	2.53759E-05	2.21416E-05	2.13238E-08	2.36211E-09
21	8.71921E-04	1.95179E-02	0.00000E+00	2.52694E-05	2.19443E-05	2.12955E-08	2.35983E-09
22	8.78022E-04	1.94415E-02	0.00000E+00	2.50441E-05	2.15239E-05	2.12624E-08	2.35709E-09
23	8.82603E-04	1.94121E-02	0.00000E+00	2.47645E-05	2.09992E-05	2.12257E-08	2.35433E-09
24	8.85661E-04	1.94240E-02	0.00000E+00	2.44902E-05	2.04852E-05	2.12242E-08	2.35378E-09
25	8.88720E-04	1.94704E-02	0.00000E+00	2.41130E-05	1.97686E-05	2.11010E-08	2.34650E-09

Figure 3-40. Group One LFPA Isotope Cross Section Differences for Cubic Spline Fit in Verification Test #19

...	EDIT OF (FISSIONABLE) COMPOSITION FL11E									
0	ICHI = -1									
0	GROUP	ABSORPTION	TOTAL	REMOVAL	TRANSPORT	FISSION	NU*FISSION	CHI	NUP	NDN
	1	3.098604E-03	1.872179E-01	2.165476E-02	1.172630E-01	2.509003E-03	6.908350E-03	7.654490E-01	6	0
	2	2.938382E-03	2.673692E-01	4.589983E-03	1.903871E-01	1.472946E-03	3.605150E-03	2.343930E-01	5	1
	3	5.941315E-02	2.229130E-01	6.007301E-02	2.118749E-01	1.961408E-02	4.773679E-02	1.602830E-04	4	2
	4	4.449683E-02	1.600869E-01	4.831201E-02	1.578014E-01	3.243415E-02	7.900407E-02	0.000000E+00	3	3
	5	1.384201E-01	2.552850E-01	1.472690E-01	2.529815E-01	1.117374E-01	2.722704E-01	0.000000E+00	2	4
	6	2.650905E-01	3.814249E-01	2.738659E-01	3.791968E-01	2.170723E-01	5.289401E-01	0.000000E+00	1	5
	7	5.760510E-01	6.903818E-01	5.840729E-01	6.880675E-01	4.749500E-01	1.157311E+00	0.000000E+00	0	6
...										

Figure 3-41. REBUS-PC Macroscopic Cross Section Output Excerpt of Verification Test #19

Fission Cross Sections from REBUSPC Output for Fuel Composition in Region FL11E							
TimeNode / Group	1	2	3	4	5	6	7
0	2.50900E-03	1.47295E-03	1.96141E-02	3.24342E-02	1.11737E-01	2.17072E-01	4.74950E-01
1	2.49999E-03	1.45918E-03	1.94416E-02	3.21175E-02	1.11636E-01	2.14213E-01	4.69369E-01
2	2.49107E-03	1.44539E-03	1.92681E-02	3.18063E-02	1.11563E-01	2.12525E-01	4.65325E-01
3	2.48219E-03	1.43162E-03	1.90948E-02	3.14957E-02	1.11470E-01	2.10863E-01	4.61304E-01
4	2.47329E-03	1.41788E-03	1.89217E-02	3.11846E-02	1.11354E-01	2.09222E-01	4.57304E-01
5	2.46440E-03	1.40417E-03	1.87490E-02	3.08734E-02	1.11218E-01	2.07602E-01	4.53329E-01
6	2.45554E-03	1.39038E-03	1.85744E-02	3.05627E-02	1.11064E-01	2.05978E-01	4.49338E-01
7	2.44668E-03	1.37665E-03	1.84008E-02	3.02517E-02	1.10888E-01	2.04340E-01	4.45338E-01
8	2.43781E-03	1.36300E-03	1.82288E-02	2.99401E-02	1.10690E-01	2.02690E-01	4.41337E-01
9	2.42895E-03	1.34937E-03	1.80568E-02	2.96287E-02	1.10473E-01	2.01038E-01	4.37340E-01
10	2.42010E-03	1.33576E-03	1.78850E-02	2.93175E-02	1.10238E-01	1.99394E-01	4.33359E-01

Fission Cross Sections from MATLAB Calculation for Fuel Composition in Region FL11E							
TimeNode / Group	1	2	3	4	5	6	7
0	2.50900E-03	1.47295E-03	1.96141E-02	3.24342E-02	1.11737E-01	2.17073E-01	4.74951E-01
1	2.49998E-03	1.45918E-03	1.94416E-02	3.21175E-02	1.11636E-01	2.14213E-01	4.69369E-01
2	2.49107E-03	1.44539E-03	1.92681E-02	3.18063E-02	1.11563E-01	2.12525E-01	4.65325E-01
3	2.48219E-03	1.43162E-03	1.90948E-02	3.14957E-02	1.11469E-01	2.10863E-01	4.61304E-01
4	2.47329E-03	1.41788E-03	1.89217E-02	3.11846E-02	1.11354E-01	2.09222E-01	4.57304E-01
5	2.46440E-03	1.40417E-03	1.87490E-02	3.08734E-02	1.11217E-01	2.07602E-01	4.53329E-01
6	2.45554E-03	1.39038E-03	1.85744E-02	3.05627E-02	1.11064E-01	2.05978E-01	4.49338E-01
7	2.44667E-03	1.37665E-03	1.84008E-02	3.02517E-02	1.10888E-01	2.04340E-01	4.45337E-01
8	2.43781E-03	1.36300E-03	1.82288E-02	2.99401E-02	1.10690E-01	2.02690E-01	4.41337E-01
9	2.42895E-03	1.34937E-03	1.80568E-02	2.96287E-02	1.10473E-01	2.01038E-01	4.37340E-01
10	2.42011E-03	1.33576E-03	1.78850E-02	2.93175E-02	1.10238E-01	1.99394E-01	4.33359E-01

Figure 3-42. Macroscopic Fission Cross Section in Region FL11E for Cubic Spline Fit in Verification Test #19

Verification test #18 uses the linear interpolation scheme for cross section data. Figure 3-43 provides an excerpt of the A.BURN input. A comparison of this input to verification test #19 in Figure 3-36 shows only the type 40 input cards are impacted.

BURNUP DEPENDENT XS DATA FOR U38A_0, DEPENDING ON U35A_0 NUMBER DENSITY									
26	U35A_0U38A_0								
39	U35A_0	1	7U38A_0	1	7PU9A_0	1	7		
39	U35C_0	1	7U38C_0	1	7PU9C_0	1	7		
39	LFP A_0	1	7LFPC_0	1	7				
40	U38A_0	11	1.0-3	8U38A_0	12	1.0-3	8		
41	U38A_0U38A_0	8.90249E-04		1.0+3	U38A_1	8.87191E-04		1.0	
41	U38A_0U38A_2	8.84131E-04		1.0	U38A_3	8.81076E-04		1.0	
41	U38A_0U38A_4	8.74968E-04		1.0	U38A_5	8.68874E-04		1.0	
41	U38A_0U38A_6	8.65830E-04		1.0	U38A_7	8.53699E-04		1.0	
41	U38A_0U38A_8	8.41609E-04		1.0	U38A_9	8.29566E-04		1.0	
41	U38A_0U38A10	8.23559E-04		1.0	U38A11	7.99701E-04		1.0	
41	U38A_0U38A12	7.76015E-04		1.0	U38A13	7.52494E-04		1.0	
41	U38A_0U38A14	7.40798E-04		1.0	U38A15	6.94709E-04		1.0	
41	U38A_0U38A16	6.49282E-04		1.0	U38A17	6.04544E-04		1.0	
41	U38A_0U38A18	5.82434E-04		1.0	U38A19	4.97058E-04		1.0	
41	U38A_0U38A20	4.14788E-04		1.0	U38A21	3.35994E-04		1.0	
41	U38A_0U38A22	2.98069E-04		1.0	U38A23	2.28978E-04		1.0	
41	U38A_0U38A24	1.65557E-04		1.0	U38A25	1.09277E-04		1.0	

Figure 3-43. REBUS-PC A.BURN Input Excerpt for Verification Test #18

The exact same approach to check capability #11 was carried out for capability #12. The piecewise linear polynomial interpolation scheme was implemented in a MATLAB program that is provided in the repository. The region isotopic densities and macroscopic cross sections were extracted from POLYFI.BCD and the REBUS-PC output. The interpolated cross sections of REBUS-PC and MATLAB were written to ASCII files with the same formats, and the resulting files were compared. Using the piecewise linear polynomial fit of microscopic cross section data, the fission cross sections of each fuel composition were tabulated at the same eleven time nodes as in verification test #19.

Figure 3-44 compares the burnup dependent cross sections for the first energy group of the lumped fission product isotope LFP A_0. The upper section is taken from REBUS-PC while the lower section was calculated with MATLAB. As was the case with verification test #19, the lines with differences are highlighted along with the actual numbers that are different on each line. Once again, errors only appear in the final significant digit, which is within the error of the math precision being performed in REBUS-PC. Extensive checking of all of the isotopic cross data was done and only found errors of this order, which are a result of the math precision in REBUS-PC.

Figure 3-45 provides an excerpt of the REBUS-PC output for the macroscopic cross sections. A quick comparison of these cross sections with those obtained with cubic spline shows they are very similar, with errors slightly larger than the last significant digit. These differences are attributable to the different interpolation scheme providing more evidence that the REBUS-PC input is being processed and used as expected. For completeness, a MATLAB program was used to calculate the macroscopic cross sections and display the condensed results for fission in Figure 3-46 for region FL11E. A quick survey of these results shows that the errors only appear in the final significant digit, which is attributable to the precision in REBUS-PC.

Additional comparisons for other regions and reactions were done and found with similar errors. As a consequence of this work, the piecewise linear spline routine of REBUS-PC was demonstrated to correctly perform the cross section interpolation consistent with that described in the manual, thus satisfying capability 12. As was the case for verification test #19, the isotopes specified in the ISOTXS file are properly linked to the region of interest, thereby verifying capability 3.

REBUSPC-interpolated XS in group 1 for isotope LFPA_0							
	X	CAPTURE	FISSION	N, P	N, ALPHA	N, D	N, T
1	1.37417E-04	1.76430E-02	0.00000E+00	2.29220E-05	1.80222E-05	2.64531E-08	2.57348E-09
2	1.97267E-04	1.81078E-02	0.00000E+00	2.34875E-05	1.89524E-05	2.57735E-08	2.56880E-09
3	2.63523E-04	1.85208E-02	0.00000E+00	2.39891E-05	1.97614E-05	2.51595E-08	2.56076E-09
4	3.17032E-04	1.87865E-02	0.00000E+00	2.43108E-05	2.02952E-05	2.46983E-08	2.55007E-09
5	3.75391E-04	1.89820E-02	0.00000E+00	2.45442E-05	2.07279E-05	2.42009E-08	2.53071E-09
6	4.55923E-04	1.92228E-02	0.00000E+00	2.48343E-05	2.12511E-05	2.35955E-08	2.50484E-09
7	5.39746E-04	1.94487E-02	0.00000E+00	2.51125E-05	2.17223E-05	2.30742E-08	2.48022E-09
8	5.93489E-04	1.95791E-02	0.00000E+00	2.52759E-05	2.19932E-05	2.27706E-08	2.46450E-09
9	6.26913E-04	1.96353E-02	0.00000E+00	2.53461E-05	2.21240E-05	2.25790E-08	2.45250E-09
10	6.71996E-04	1.97102E-02	0.00000E+00	2.54377E-05	2.22890E-05	2.23327E-08	2.43648E-09
11	7.17754E-04	1.97876E-02	0.00000E+00	2.55306E-05	2.24444E-05	2.21025E-08	2.42100E-09
12	7.46646E-04	1.98338E-02	0.00000E+00	2.55846E-05	2.25330E-05	2.19602E-08	2.41113E-09
13	7.64254E-04	1.98512E-02	0.00000E+00	2.56030E-05	2.25690E-05	2.18663E-08	2.40407E-09
14	7.87858E-04	1.98691E-02	0.00000E+00	2.56224E-05	2.26062E-05	2.17418E-08	2.39465E-09
15	8.11630E-04	1.98722E-02	0.00000E+00	2.56322E-05	2.26199E-05	2.16208E-08	2.38546E-09
16	8.26563E-04	1.98617E-02	0.00000E+00	2.56295E-05	2.26120E-05	2.15454E-08	2.37968E-09
17	8.35588E-04	1.98325E-02	0.00000E+00	2.56095E-05	2.25779E-05	2.14951E-08	2.37566E-09
18	8.47654E-04	1.97697E-02	0.00000E+00	2.55638E-05	2.24957E-05	2.14284E-08	2.37032E-09
19	8.59765E-04	1.96653E-02	0.00000E+00	2.54687E-05	2.23165E-05	2.13642E-08	2.36530E-09
20	8.67352E-04	1.95809E-02	0.00000E+00	2.53741E-05	2.21383E-05	2.13236E-08	2.36209E-09
21	8.71921E-04	1.95187E-02	0.00000E+00	2.52582E-05	2.19233E-05	2.12963E-08	2.35987E-09
22	8.78022E-04	1.94473E-02	0.00000E+00	2.50221E-05	2.14821E-05	2.12592E-08	2.35690E-09
23	8.82603E-04	1.94155E-02	0.00000E+00	2.47552E-05	2.09821E-05	2.12299E-08	2.35456E-09
24	8.85661E-04	1.94285E-02	0.00000E+00	2.44768E-05	2.04591E-05	2.12083E-08	2.35290E-09
25	8.88720E-04	1.94725E-02	0.00000E+00	2.41053E-05	1.97525E-05	2.10798E-08	2.34533E-09

MATLAB-interpolated XS in group 1 for isotope LFPA_0							
	X	CAPTURE	FISSION	N, P	N, ALPHA	N, D	N, T
1	1.37417E-04	1.76429E-02	0.00000E+00	2.29220E-05	1.80223E-05	2.64532E-08	2.57348E-09
2	1.97267E-04	1.81079E-02	0.00000E+00	2.34875E-05	1.89524E-05	2.57736E-08	2.56881E-09
3	2.63523E-04	1.85208E-02	0.00000E+00	2.39891E-05	1.97613E-05	2.51596E-08	2.56076E-09
4	3.17032E-04	1.87865E-02	0.00000E+00	2.43108E-05	2.02952E-05	2.46983E-08	2.55007E-09
5	3.75391E-04	1.89820E-02	0.00000E+00	2.45442E-05	2.07278E-05	2.42008E-08	2.53071E-09
6	4.55923E-04	1.92229E-02	0.00000E+00	2.48343E-05	2.12512E-05	2.35954E-08	2.50483E-09
7	5.39746E-04	1.94487E-02	0.00000E+00	2.51126E-05	2.17223E-05	2.30742E-08	2.48021E-09
8	5.93489E-04	1.95791E-02	0.00000E+00	2.52759E-05	2.19933E-05	2.27707E-08	2.46450E-09
9	6.26913E-04	1.96353E-02	0.00000E+00	2.53462E-05	2.21239E-05	2.25791E-08	2.45250E-09
10	6.71996E-04	1.97101E-02	0.00000E+00	2.54375E-05	2.22891E-05	2.23328E-08	2.43649E-09
11	7.17754E-04	1.97877E-02	0.00000E+00	2.55305E-05	2.24445E-05	2.21025E-08	2.42101E-09
12	7.46646E-04	1.98339E-02	0.00000E+00	2.55846E-05	2.25330E-05	2.19602E-08	2.41113E-09
13	7.64254E-04	1.98512E-02	0.00000E+00	2.56029E-05	2.25690E-05	2.18662E-08	2.40407E-09
14	7.87858E-04	1.98691E-02	0.00000E+00	2.56224E-05	2.26061E-05	2.17417E-08	2.39464E-09
15	8.11630E-04	1.98722E-02	0.00000E+00	2.56322E-05	2.26200E-05	2.16209E-08	2.38546E-09
16	8.26563E-04	1.98617E-02	0.00000E+00	2.56296E-05	2.26120E-05	2.15454E-08	2.37969E-09
17	8.35588E-04	1.98325E-02	0.00000E+00	2.56095E-05	2.25779E-05	2.14950E-08	2.37565E-09
18	8.47654E-04	1.97697E-02	0.00000E+00	2.55638E-05	2.24956E-05	2.14285E-08	2.37034E-09
19	8.59765E-04	1.96653E-02	0.00000E+00	2.54687E-05	2.23165E-05	2.13642E-08	2.36529E-09
20	8.67352E-04	1.95809E-02	0.00000E+00	2.53741E-05	2.21384E-05	2.13237E-08	2.36210E-09
21	8.71921E-04	1.95187E-02	0.00000E+00	2.52583E-05	2.19234E-05	2.12963E-08	2.35988E-09
22	8.78022E-04	1.94472E-02	0.00000E+00	2.50220E-05	2.14821E-05	2.12592E-08	2.35690E-09
23	8.82603E-04	1.94156E-02	0.00000E+00	2.47553E-05	2.09822E-05	2.12300E-08	2.35457E-09
24	8.85661E-04	1.94285E-02	0.00000E+00	2.44769E-05	2.04591E-05	2.12083E-08	2.35291E-09
25	8.88720E-04	1.94725E-02	0.00000E+00	2.41052E-05	1.97526E-05	2.10798E-08	2.34532E-09

Figure 3-44. Group One LFPA Isotope Cross Section Differences for a Piecewise Linear Fit in Verification Test #18

...	EDIT OF (FISSIONABLE) COMPOSITION FL11E									
0										
	ICHI = -1									
0	GROUP	ABSORPTION	TOTAL	REMOVAL	TRANSPORT	FISSION	NU*FISSION	CHI	NUP	NDN
	1	3.098604E-03	1.872179E-01	2.165476E-02	1.172630E-01	2.509003E-03	6.908350E-03	7.654490E-01	6	0
	2	2.938381E-03	2.673692E-01	4.589982E-03	1.903871E-01	1.472945E-03	3.605149E-03	2.343930E-01	5	1
	3	5.941313E-02	2.229130E-01	6.007299E-02	2.118749E-01	1.961408E-02	4.773679E-02	1.602830E-04	4	2
	4	4.449684E-02	1.600869E-01	4.831202E-02	1.578014E-01	3.243415E-02	7.900408E-02	0.000000E+00	3	3
	5	1.384202E-01	2.552850E-01	1.472690E-01	2.529815E-01	1.117374E-01	2.722706E-01	0.000000E+00	2	4
	6	2.650926E-01	3.814249E-01	2.738680E-01	3.791968E-01	2.170741E-01	5.289445E-01	0.000000E+00	1	5
	7	5.760538E-01	6.903818E-01	5.840757E-01	6.880675E-01	4.749524E-01	1.157317E+00	0.000000E+00	0	6...

Figure 3-45. REBUS-PC Macroscopic Cross Section Output Excerpt of Verification Test #18

Fission Cross Sections from REBUSPC Output for Fuel Composition in Region FL11E								
TimeNode / Group	1	2	3	4	5	6	7	
0	2.50900E-03	1.47295E-03	1.96141E-02	3.24342E-02	1.11737E-01	2.17074E-01	4.74952E-01	
1	2.49999E-03	1.45918E-03	1.94416E-02	3.21175E-02	1.11636E-01	2.14216E-01	4.69372E-01	
2	2.49107E-03	1.44539E-03	1.92681E-02	3.18063E-02	1.11563E-01	2.12525E-01	4.65324E-01	
3	2.48219E-03	1.43163E-03	1.90949E-02	3.14956E-02	1.11470E-01	2.10867E-01	4.61308E-01	
4	2.47329E-03	1.41788E-03	1.89217E-02	3.11846E-02	1.11354E-01	2.09223E-01	4.57305E-01	
5	2.46441E-03	1.40416E-03	1.87488E-02	3.08734E-02	1.11218E-01	2.07603E-01	4.53329E-01	
6	2.45554E-03	1.39038E-03	1.85745E-02	3.05626E-02	1.11064E-01	2.05977E-01	4.49336E-01	
7	2.44668E-03	1.37665E-03	1.84009E-02	3.02516E-02	1.10888E-01	2.04340E-01	4.45338E-01	
8	2.43781E-03	1.36300E-03	1.82288E-02	2.99397E-02	1.10692E-01	2.02695E-01	4.41345E-01	
9	2.42895E-03	1.34937E-03	1.80568E-02	2.96283E-02	1.10475E-01	2.01046E-01	4.37351E-01	
10	2.42011E-03	1.33577E-03	1.78851E-02	2.93174E-02	1.10238E-01	1.99395E-01	4.33361E-01	

Fission Cross Sections from MATLAB Calculation for Fuel Composition in Region FL11E								
TimeNode / Group	1	2	3	4	5	6	7	
0	2.50900E-03	1.47295E-03	1.96141E-02	3.24342E-02	1.11737E-01	2.17074E-01	4.74953E-01	
1	2.49998E-03	1.45918E-03	1.94416E-02	3.21175E-02	1.11636E-01	2.14216E-01	4.69372E-01	
2	2.49107E-03	1.44539E-03	1.92681E-02	3.18063E-02	1.11563E-01	2.12525E-01	4.65324E-01	
3	2.48219E-03	1.43163E-03	1.90949E-02	3.14955E-02	1.11470E-01	2.10867E-01	4.61308E-01	
4	2.47329E-03	1.41788E-03	1.89217E-02	3.11847E-02	1.11354E-01	2.09224E-01	4.57305E-01	
5	2.46440E-03	1.40416E-03	1.87488E-02	3.08734E-02	1.11218E-01	2.07603E-01	4.53329E-01	
6	2.45554E-03	1.39038E-03	1.85745E-02	3.05626E-02	1.11064E-01	2.05977E-01	4.49337E-01	
7	2.44667E-03	1.37665E-03	1.84009E-02	3.02516E-02	1.10888E-01	2.04339E-01	4.45338E-01	
8	2.43781E-03	1.36300E-03	1.82288E-02	2.99397E-02	1.10691E-01	2.02695E-01	4.41345E-01	
9	2.42895E-03	1.34937E-03	1.80568E-02	2.96283E-02	1.10475E-01	2.01046E-01	4.37351E-01	
10	2.42011E-03	1.33576E-03	1.78851E-02	2.93174E-02	1.10238E-01	1.99395E-01	4.33361E-01	

Figure 3-46. Macroscopic Fission Cross Section in Region FL11E for Piecewise Linear Fit in Verification Test #18

Although not stated in the list of capabilities, the polynomial approximation must also be verified, which is verification test #20. This feature is employed by active users of REBUS-PC and thus the same comparisons of verification tests #18 and #19 were done for completeness. The outcome is the same, in that the MATLAB program yielded identical macroscopic cross sections at each time node. For brevity, the comparison results are not entirely displayed in this manuscript.

Although not part of the capability verification process, a comparison of the three different cross section interpolation schemes in REBUS-PC is provided for the STRZ benchmark problem. Table 3-27 provides the k-effective results obtained for each time step using a cubic spline, piecewise linear polynomial and eighth order polynomial fit of the cross section data.

Table 3-27. REBUS-PC K-effective Results for Different Cross Section Interpolation Schemes

Time Node	k-effective Results			Difference	
	Cubic Spline	Piecewise Linear	8 th Order Polynomial	Piecewise Linear - Spline	8 th Order Polynomial - Spline
0	1.09918 63	1.09918 75	1.09917 02	0.00000 13	-0.00001 60
1	1.05116 79	1.05116 93	1.05154 22	0.00000 14	0.00037 42
2	1.04633 26	1.04632 26	1.04646 49	-0.00000 99	0.00013 23
3	1.04251 66	1.04250 73	1.04250 31	-0.00000 93	-0.00001 36
4	1.03944 78	1.03943 67	1.03935 40	-0.00001 11	-0.00009 39
5	1.03682 55	1.03681 10	1.03670 79	-0.00001 45	-0.00011 76
6	1.03443 78	1.03442 68	1.03433 57	-0.00001 10	-0.00010 22
7	1.03216 46	1.03215 48	1.03209 98	-0.00000 98	-0.00006 48
8	1.02994 21	1.02993 08	1.02992 34	-0.00001 13	-0.00001 87
9	1.02773 63	1.02772 92	1.02776 43	-0.00000 71	0.00002 80
10	1.02553 04	1.02552 27	1.02559 94	-0.00000 77	0.00006 90

The cubic spline and piecewise linear polynomial options yield very similar results, with errors near the convergence tolerance set for the flux and depletion solver. The 8th order polynomial fit yields noticeably different results at several time nodes from those obtained with the other two options. The k-effective difference shown here can be considered a measure of the reactivity uncertainty introduced by the cross section fitting scheme. Because of the known approximations that the polynomial approximation introduces, it is strongly advised to use one of the other two approximations, although it is noted that all of these errors will have a minor impact on the computed results.

As was the case with the microscopic cross section comparisons, the differences between the REBUS-PC and MATLAB calculations only appear in the sixth significant digit, which is within the limits of the math precision of REBUS-PC. Additional comparisons were made for other regions and reactions and found similar errors. As a consequence, the piecewise linear fit routine of REBUS-PC is shown to correctly perform the cross section interpolation, consistent with that described in the manual and thus satisfies capability #12. In addition, the isotopes specified in the ISOTXS file are shown to be properly linked to the region of interest, thereby verifying capability 3. This work additionally verifies the polynomial fit of burnup-dependent cross sections in REBUS-PC, although this is not listed as a capability.

In summary, the preceding verification tests demonstrate the following capabilities:

- Capability 3 is partially satisfied, as the ISOTXS isotope cross section data and depletion results were demonstrated to be correctly linked to the region and composition input.
- Capability 11, as the cubic spline cross section interpolation scheme was verified against a MATLAB equivalent to six significant digits.
- Capability 11, as the piecewise linear cross section interpolation scheme was verified against a MATLAB equivalent to six significant digits.

3.14 Verification Test #21 and #22

To finalize verification of capability 3, the depletion calculation itself needs to be demonstrated to be accurate and based upon the input. The depletion solver in REBUS-PC is accurate has extensive historical use and validation. To verify capability 3, the depletion chain is simplified and an analytic flux solution is used so that the accuracy of the REBUS-PC solution can be shown mathematically. This is verification test #21, which is based upon the 1GCVL_hom described geometry. MATLAB was used to provide the reference solution.

Table 3-28 provides the depletion chain information used in verification test #21. The REBUS-PC input that implements it is shown in Figure 3-47. From inspection of the REBUS-PC input, one can also identify the cross section data shown in Table 3-28 for verification test #21 as the data is provided in the A.ISO format. The isotope LUMP represents a lumped fission product and the isotope DUMP is used as a fictitious isotope to terminate burn chains. The yield fractions of the lumped fission products are omitted as it should be clear that one LUMP is produced per fission. It is noted that there is some absorption in the LUMP and DUMP isotopes, as can be seen in Table 3-28.

Table 3-28. Depletion Chain Setup for Verification Test #21

Isotope	Reaction	Product Isotope	Cross Sections (barn)	Decay Constant (s ⁻¹)
U-235	n, γ	DUMP	1.15810E+01	
	n, f	LUMP	5.41443E+01	
	n, 2n	DUMP	4.27508E-03	
U-238	n, γ	Pu-239	1.89742E+00	
	n, f	LUMP	1.18442E-01	
	n, 2n	DUMP	5.17885E-03	
Pu-239	n, γ	DUMP	5.73755E+01	
	n, f	LUMP	1.11015E+02	
	n, 2n	DUMP	2.28699E-03	
	α decay	U-235		9.120E-05
LUMP	n, γ	LUMP	2.59800E+01	
	n, 2n	LUMP	1.28623E-03	
	β - decay	LUMP		1.526E-08
	α decay	LUMP		1.027E-13
DUMP	n, γ	DUMP	1.84494E-01	
	n, α	DUMP	8.25215E+00	

...				
DATASET=A.BURN				
...				
09	U235	1	DUMP	
09	U235	2	LUMP	1.
09	U235	5	DUMP	
09	U238	1	PU239	
09	U238	2	LUMP	1.
09	U238	5	DUMP	
09	PU239	1	DUMP	
09	PU239	2	LUMP	1.
09	PU239	5	DUMP	
09	PU239	8	U235	
09	LUMP	1	LUMP	
09	LUMP	5	LUMP	
09	LUMP	6	LUMP	
09	LUMP	8	LUMP	
09	DUMP	1	DUMP	
09	DUMP	4	DUMP	
25	LUMP	6	LUMP	1.526-08
25	LUMP	8	LUMP	1.027-13
25	PU239	8	U235	9.120-05
...				

Figure 3-47. A.BURN Depletion Chain Excerpt for Verification Test #21

In this verification test, the power level was set to 10 MW, which yields a one-group average flux level of $2.6713 \cdot 10^{16}$ neutrons/cm²·s. When combined with a one-day burn step and one-day decay step, the nuclide depletion from both neutron reactions and radioactive decays can be tested. The system of depletion equations can be written in a matrix form as:

$$\frac{\partial}{\partial t} \begin{bmatrix} N_{U25} \\ N_{U28} \\ N_{P49} \\ N_{LP} \\ N_{DP} \end{bmatrix} = \begin{bmatrix} -A_{U25} & 0 & \lambda^{P49} & 0 & 0 \\ 0 & -A_{U28} & 0 & 0 & 0 \\ 0 & \sigma_{n,\gamma}^{U28} \phi & -A_{P49} & 0 & 0 \\ \sigma_{n,f}^{U25} \phi & \sigma_{n,f}^{U28} \phi & \sigma_{n,f}^{P49} \phi & 0 & 0 \\ (\sigma_{n,\gamma}^{U25} + \sigma_{n,2n}^{U25}) \phi & \sigma_{n,2n}^{U28} \phi & (\sigma_{n,\gamma}^{P49} + \sigma_{n,2n}^{P49}) \phi & 0 & 0 \end{bmatrix} \begin{bmatrix} N_{U25} \\ N_{U28} \\ N_{P49} \\ N_{LP} \\ N_{DP} \end{bmatrix} \quad (10)$$

where

$$A_{U25} = (\sigma_{n,\gamma}^{U25} + \sigma_{n,f}^{U25} + \sigma_{n,2n}^{U25}) \phi \quad (11)$$

$$A_{U28} = (\sigma_{n,\gamma}^{U28} + \sigma_{n,f}^{U28} + \sigma_{n,2n}^{U28}) \phi \quad (12)$$

$$A_{P49} = (\sigma_{n,\gamma}^{P49} + \sigma_{n,f}^{P49} + \sigma_{n,2n}^{P49}) \phi + \lambda^{P49} \quad (13)$$

In equation 10, N_{xx} denotes the nuclide atom density, while the subscripts $U25$, $U28$, $P49$, LP , and DP denote U-235, U-238, Pu-239, lumped fission product, and the dump isotope, respectively. The system of equations during the shutdown time can be obtained by setting the flux to zero in equations 10 through 13.

The reference nuclide densities were calculated at the end of the burn step and at the end of the shutdown period using the nuclide densities defined at the beginning of the problem and the exponentials of the transmutation matrices during the burn step and the shutdown period. The exponentials of the transmutation matrices were calculated using the MATLAB program.

Table 3-29 compares the nuclide density solutions of REBUS-PC with the MATLAB reference solutions at the end of the burn step and at the end of the decay step. At the end of both periods, one can see that the atom density solutions of REBUS-PC agree with those of the MATLAB solution.

As a further verification, one can easily solve the decay process for a simple decaying isotope using the formula $N(t) = N(0)\exp(-\lambda t)$ and obtain the expected results for the U-235 and Pu-239 atomic densities. As an example, taking the decay constant of Pu-239, $9.120\text{E-}05\text{ s}^{-1}$, and the atom density at the end of the burn step of $1.4701\text{E-}06\text{ atoms/b-cm}$, one can calculate the Pu-239 atom density after the decay step as

$$N(t) = 1.4701 \cdot 10^{-06} \cdot \exp(-0.0000912 \cdot \text{sec}^{-1} \cdot 1 \cdot \text{day}) = 5.5622 \cdot 10^{-10} \text{ atoms/b-cm}, \quad (14)$$

which is similar to the result shown in Table 3-29 for Pu-239 within the precision of the REBUS-PC and MATLAB solutions within four significant figures (atom density of $1.4701\text{E-}06$ is not exactly the values computed in REBUSPC and MATLAB). It should be noted that the decay constants and cross sections used in this problem are not realistic, but are only defined to demonstrate the depletion chain accuracy. The results of this verification test show that REBUS-PC solves the transmutation equations correctly in both burn and decay modes. The test also verifies that the input isotopic cross section data is being used properly in the region of interest.

Table 3-29. Comparison of Atom Density (atoms/barn-cm) for Verification Test #21

Isotope	End of Burn Step		End of Decay Step	
	REBUS-PC Solution	MATLAB Reference Solution	REBUS-PC Solution	MATLAB Reference Solution
U-235	6.0658E-04	6.0658E-04	6.0805E-04	6.0805E-04
U-238	2.7747E-03	2.7747E-03	2.7747E-03	2.7747E-03
Pu-239	1.4701E-06	1.4701E-06	5.5620E-10	5.5620E-10
LUMP	8.2204E-05	8.2204E-05	8.2204E-05	8.2204E-05
DUMP	1.7560E-05	1.7560E-05	1.7560E-05	1.7560E-05

Verification test #22 is based upon the seven-group 7GXYZ_hom problem described earlier. Its purpose is to test the region-density iteration scheme in REBUS-PC. The region-density iteration scheme updates the depletion calculation over the step based on the flux solution at the beginning and end of the burn step. Nuclide depletion over a burn step is a complex problem because the neutron flux changes throughout the step due to ongoing depletion and production of each nuclide in the problem. REBUS-PC employs the approximation of a linear change in the flux solution over the burn step and solves the depletion over each burn step by computing an average transmutation matrix over the time step. Because the flux solution and atom densities at the end of the time step are connected, the region-density calculations in REBUS-PC are solved iteratively.

Figure 3-48 shows the input geometry for verification test #22, which defines an infinite homogeneous problem with three boxes. Because of the depletion, the spectrum changes over the time step, so that the averaging of the transmutation matrix becomes evident. As can be seen in Figure 3-48, the region-density extrapolation option was turned off by providing a negative number of region-density iterations on the type 02 card of the dataset A.BURN. Because this test is a burnup problem of an infinite homogeneous geometry, the REBUS-PC output produces identical nuclide densities for all three regions after each iteration.

The atom densities in each region were compared with the solution obtained using a MATLAB program that carries out the same methodology. The MATLAB nuclide densities at the end of the depletion step were also calculated using the matrix exponential method. The REBUS-PC output was examined after each region density iteration and its consistency with the MATLAB results was verified. Table 3-30 compares the atom densities in each region after each iteration.

```

...
DATASET=A.NIP3
...
03          44
04          3      3      3      3      3      3
06  FUELA  0.00000E+00 5.00000E+00      0      10 5.00000E+00 1.00000E+01
06  FUELB  5.00000E+00 1.00000E+01      0      10 5.00000E+00 1.00000E+01
06  FUELC  0.00000E+00 1.00000E+01      0      10 0.00000E+00 5.00000E+00
07  HMREG  FUELA FUELB FUELC
...
13          MEAT1 U35A_0 2.2518E-03 U38A_0 9.0341E-03 PU9A_0 1.0000E-20
13          MEAT1 LFPA_0 1.0000E-20 O16B_0 1.0000E-20
13          MODA  H01A_0 6.6691E-02 O16A_0 3.3346E-02
14          MIXA  MEAT1 3.6857E-01 MODA 6.3143E-01
14          FUEL1 MIXA 1.0
15  FUEL1  HMREG
...
DATASET=A.BURN
02          999999      0.001      0.001      0.0001      -5      5
03          0      0.0      0.0      10.0      -1.0      1      0
...
35  PATH1  FUEL1 FUELA 1      1
35  PATH2  FUEL1 FUELB 1      1
35  PATH3  FUEL1 FUELC 1      1
...

```

Figure 3-48. Input Geometry Definition for Verification Test #22

Table 3-30. Comparison of Atom Densities at Each Iteration of Verification Test #22

Iteration		U-235	U-238	Pu-239	LUMP	DUMP
BOC	REBUS-PC	8.29946E-04	3.32970E-03	0.0000E+00	0.0000E+00	0.0000E+00
	MATLAB	8.29946E-04	3.32970E-03	0.0000E+00	0.0000E+00	0.0000E+00
0th Iteration	REBUS-PC	5.52567E-04	3.25374E-03	4.11085E-05	2.44869E-04	6.73581E-05
	MATLAB	5.52567E-04	3.25374E-03	4.11085E-05	2.44869E-04	6.73581E-05
1st Iteration	REBUS-PC	5.23185E-04	3.24527E-03	4.34652E-05	2.72774E-04	7.49483E-05
	MATLAB	5.23185E-04	3.24527E-03	4.34652E-05	2.72774E-04	7.49483E-05
2nd Iteration	REBUS-PC	5.18166E-04	3.24402E-03	4.37016E-05	2.77570E-04	7.61843E-05
	MATLAB	5.18166E-04	3.24402E-03	4.37016E-05	2.77570E-04	7.61843E-05
3rd Iteration	REBUS-PC	5.17192E-04	3.24380E-03	4.37374E-05	2.78501E-04	7.64191E-05
	MATLAB	5.17192E-04	3.24380E-03	4.37374E-05	2.78501E-04	7.64192E-05
Final	REBUS-PC	5.16997E-04	3.24375E-03	4.37440E-05	2.78687E-04	7.64659E-05

From the input shown in Figure 3-48, the convergence criteria of the region-density iteration was set to 0.001, which was met for all nuclides in the burn matrix at the 4th iteration. From Table 3-30, one can see that the nuclide densities of REBUS-PC calculation agree well with the MATLAB solutions at

each iteration. A small difference occurs in the 6th significant digit for the DUMP isotope at the third iteration, which is attributable to the single precision math used in REBUS-PC. These results indicate that the region density iteration without extrapolation works properly in the REBUS-PC depletion calculation. It is very important to note that the final density information is not reported with the same number of significant digits in the standard output file and that one must obtain this data from the TYPE13.BCD auxiliary output file.

With the preceding results, verification tests #21 and #22 demonstrate the following capabilities:

- Capability 3, as it verifies that the depletion is correct and based upon the isotopes assigned to each region.
- Capability 14, as the region density iteration scheme without extrapolation was verified to be accurate.

4 Conclusions

The preceding discussion on verification tests and the results of those tests is sufficient proof that the REBUS-PC capabilities summarized in Section 1 all work as expected. In particular, the ability of the software to carry out fuel cycle analysis on θ -R-Z geometries was demonstrated producing the correct burnup, power, and isotopic depletion results. Analytic solutions were used to prove the accuracy of the finite difference spatial approximation.

Acknowledgement

This work was sponsored by the U.S. Department of Energy, Office of Material Management and Minimization in the U.S. National Nuclear Security Administration Office of Defense Nuclear Nonproliferation under Contract DE-AC02-06CH11357.

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