ANL/NSE-24/83

Verification of the PERSENT Software

Nuclear Science and Engineering Division

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Verification of the PERSENT Software

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Approval

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ABSTRACT

Ongoing commercial design activities require a thorough verification of the Argonne Reactor Computation codes be performed. DIF3D is central to this system and substantial work has been done to verify its accuracy on several identified commercial needs. This manuscript details the verification work done on PERSENT which relies upon the DIF3D code for its forward and adjoint flux solution.

Previous work identified the PERSENT features required to be verified to support commercial design activities, features of which are generally applicable to hexagonal-Z fast reactor designs. The scope of this verification effort includes verifying PERSENT's ability to correctly calculate four key quantities: perturbation worth distributions, kinetics parameters, sensitivity coefficients, and cross section uncertainty quantification. This manuscript provides the verification tasks and their results with respect to these quantities needed for commercial design activities.

For the perturbation worth distributions, hand calculations are deployed to verify the PERSENT calculated results. Similarly, hand calculation of the PERSENT computed kinetics parameters is also used to verify the PERSENT results. In both of these, the input to PERSENT is manipulated to ensure the hand calculation exactly matches the equations PERSENT is calculating. The sensitivity coefficients involve calculating the derivatives of a parameter (such as reactivity worth), with respect to the cross section data. Direct finite difference calculations with DIF3D are used to verify the PERSENT calculated results. For the uncertainty quantification, manufactured input to PERSENT is used to allow an exact hand calculation to reproduce the PERSENT calculated results.

This verification work was requested to be provided in two submissions by collaborating commercial companies. This version of the report only details the verification work done on the perturbation worth distribution and kinetics parameters. A follow-on revision to this report will include the verification work done on sensitivity coefficients and cross section uncertainty quantification aspects. The work detailed in this report verified that no significant issues were identified for PERSENT with regards to existing commercial design activities.

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1 Introduction

This report presents verification work done on the the modeling and simulation capabilities of Argonne National Laboratory's PERSENT (PERturbation and SENsitivity for Transport) code [1] that is used in modern commercial deployment reactor technologies. The requirements report [2] laid out the capabilities of PERSENT and established a set of PERSENT verification tasks necessary to verify PERSENT for usage on commercial projects. A similar path was followed for the DIF3D [3-9] software package.

PERSENT was developed by Argonne in 2012 and released in 2013. The main motivation behind constructing PERSENT was to fix two oustanding problems. The first problem deals with models with substantial leakage where any reactivity coefficients that involved changes in the leakage were known to have errors due to the use of diffusion theory. In the past, two-dimensional transport calculations were used to "correct" the 3D diffusion theory perturbation results. The second problem is that most of the sensitivity analysis was being done using 2D R-Z transport calculations with relatively little 3D capabilities available. For several reactivity coefficients, such as control rods or sample worths, using R-Z was known to introduce considerable errors in the sensitivity analysis work. The PERSENT code resolved these problems by building upon the DIF3D-VARIANT solver capability. At its core, DIF3D-VARIANT is a rigorous treatment of the diffusion equation. The ability of DIF3D-VARIANT to apply low order P_N transport to full core reactor problems in a reasonable amount of time, eliminates the need to do comparative R-Z transport calculations. At this time, PERSENT is still the only deterministic 3D transport capability available today for generating sensitivity coeffiicents in the world.

The requirements document [2] discusses the outputs from PERSENT used by engineers in commercial projects. This produced a set of tasks to accomplish as part of the verification work which is summarized in Table 1-1. To satisfy each task, at least one verification problem will need to be identified or created such that it can be regularly executed to verify the PERSENT software capabilities.

Table 1-1 has been organized into six categories according to the type of work and checking that needs to be done. In the first category, the DIF3D usage by PERSENT is verified by comparing the standalone DIF3D calculation with the PERSENT executed one. The DIF3D verification itself was provided elsewhere [3] thereby eliminating any need to check the accuracy of the DIF3D results in this manuscript. In the second category, the perturbation option is checked such that the perturbed inputs constructed by PERSENT are consistent with the ones desired. In the third category, the first order perturbation theory capabilities are verified. The fourth category verifies the kinetics parameter details. The second through the fourth categories are all internally connected in the PERSENT software and verifiable with hand calculations.

The fifth category focuses on checking the sensitivity calculations of PERSENT which are a series of separate subroutines and thus each sensitivity option needs to be checked individually. This category will take the most effort to verify as there are so many different options to check and each sensitivity coefficient requires a series of DIF3D calculations to verify its accuracy. The sixth category is a follow on step after sensitivity to calculate the parameter uncertainty due to cross section errors. The UQ capability is rather easy to verify as it is a simple matrix-vector product operation for a given sensitivity vector. Together, the set of verification test problems

created from this work will ensure users that the PERSENT software, if used consistently with the manual, will produce accurate results.

Table 1-1. PERSENT Identified Verification Tasks

Category	Verification Tasks
1	Verify DIF3D usage in PERSENT a) Steady state eigenvalue problem is consistent with user input b) Desired PERSENT auxiliary DIF3D controls are obeyed
2	Verify exact perturbation theory calculations a) The correct DIF3D solutions are generated b) The spatial distribution of worth is correct c) The isotopic mass change is correct d) The worth/kg result is correct e) The region and area tables are correct integrals of the mesh-wise tables
3	Verify first order perturbation theory calculations a) The worth calculation is consistent with a small exact perturbation b) The spatial distribution of worth is correct c) The worth/kg result is correct d) The bowing worth calculation is correct
4	Verify the kinetics parameter calculation is correct a) The Λ calculation is correct b) The β calculation is correct c) The coalesced kinetics parameters are consistent with the full set
5	Verify the sensitivity calculations a) The unique isotope set is generated properly b) The eigenvalue sensitivity vector is correct c) The reactivity worth sensitivity vector is correct d) The Λ sensitivity vector is correct e) The β sensitivity vector is correct f) The reaction rate ratio sensitivity vector is correct g) The inhomogeneous fixed source solver controls are obeyed h) The sensitivity vector load and store operations are correct i) The sensitivity_diff functionality is correct
6	Verify the UQ calculations a) The covariance matrix is properly loaded b) The user mapping of isotope data to the covariance data is obeyed c) The covariance matrix vector product is correct d) The isotope/reaction to isotope/reaction table is correct e) The isotope to isotope table is correct f) The reaction by isotope table is correct g) The calculation using imported sensitivity files is correct

2 Software Verification Work for PERSENT

This section is focused on summarizing the verification work for PERSENT. As part of that work, several of the following tests use independent DIF3D verification as reference solutions and thus tests were added to the DIF3D verification test suite in addition to those being created here for the PERSENT testing. The set of verification test problems is summarized at the end of this report and a table is provided linking each verification test problem to the sections of the report where they are discussed and the categories they deal with.

2.1 DIF3D Consistency Verification Test Problem

The first verification test problem is focused on demonstrating that, for each perturbation, the PERSENT outputted DIF3D results can be identically produced by independent DIF3D calculations. This set of test problems is not concerned with the accuracy of the PERSENT specific outputs.

The base of this verification test problem is a three group cross section set created in the early 1980s for use in testing the ARC software. It includes elemental data for sodium, iron, oxygen, carbon and actinide data for U-238, Pu-239, Pu-240, and Pu-241 along with a LFP and DUMP isotope typical in depletion calculations. It also has a companion DLAYXS file with it such that the kinetics parameters can be calculated. The geometry configuration is rather simplistic and pictorially represented in Figure 2-1. There are seven geometric regions shown although each control rod is separately identified by including five additional different geometric regions. All of the control regions were also setup with different axial insertion points to better display the impacts of axially inserted control rods. The remaining core regions are standard for breeder type reactors which is consistent with the original purpose of the cross section set although not important for the present work.

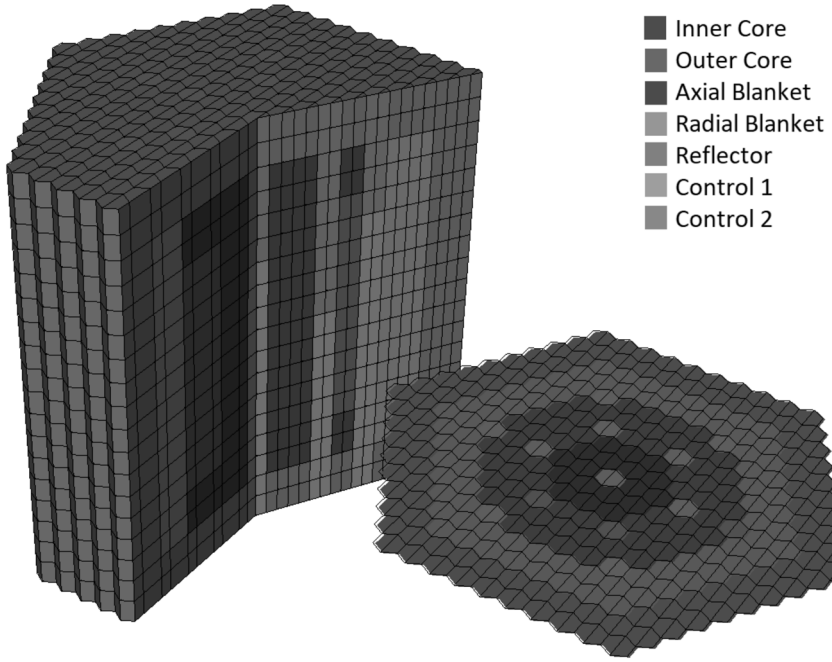

Figure 2-1. The 3D Hexagonal Test Geometry for the DIF3D Consistency Check

For the default configuration of this test problem, the control rod regions are not filled with control material (B-10) such that DIF3D produces a radially and axially symmetric solution. The power distribution is shown in Figure 2-2 to better display this symmetric spatial detail. Because the geometry is radially symmetric, the 60 degree periodic, 120 degree periodic, and full core geometry models in DIF3D-VARIANT should all produce the same result which was verified as part of the DIF3D verification process [3].

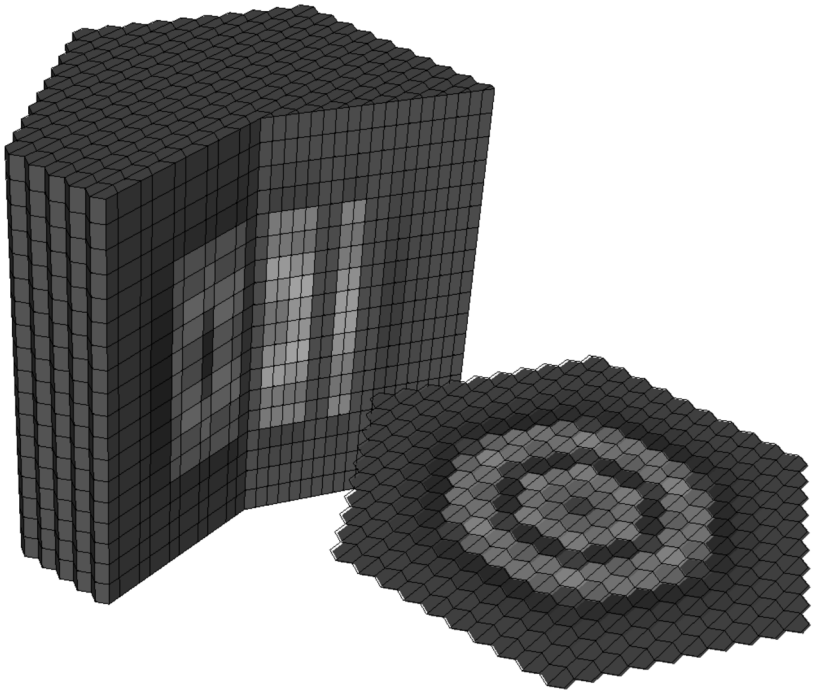

Figure 2-2. The 3D Hexagonal Power Distribution for the DIF3D Consistency Check

Figure 2-3 provides the A.NIP3 excerpt from the input model which shows how the problem in Figure 2-1 is defined. Of particular importance is how the geometry was defined. From Figure 2-1 and Figure 2-3, one can see that five control rods are defined to create thirteen hexagonal positions. Each control rod position is assigned two unique regions with two different axial heights. Two distinct materials are then created for each control rod which are assigned to the control rod regions (EMPTY1 is assigned to ROD1A, EMPTY2 is assigned to ROD2A, etc…). Finally, a single control rod material (ROD) is defined.

The regions must be defined this way to allow the control material to be defined uniquely for each control rod position. What is not required in a perturbation approach with DIF3D is the additional materials (NOROD1, NOROD2, …). To impose the perturbation in DIF3D, one can just assign material ROD and NOROD to get the desired control rod pattern to define the perturbed state (via card type 15) and thus only three materials are needed to define all of the possible control rod perturbations (NOROD, EMPTY, ROD). PERSENT only allows modifications to the zones such that one can swap zone NOROD1 with zone ROD. If NOROD1 is assigned to multiple regions, then all regions will be perturbed instead of just the single region. There is of course no zone or region constraint with regard to applying the perturbation or sensitivity operations, but with the stated zone replacement strategy in PERSENT, the user input might have to be modified

to allow the desired perturbation as was done here. For regular perturbation theory calculations (fuel, structure, sodium density, sodium void, axial expansion, etc…), this issue is entirely unimportant.

```
…
03  120
04  4  4  4  4  4  4

09 Z  2  20.0  $ Lower struct
09 Z  2  40.0  $ Lower blanket
09 Z 10 140.0  $ active core
09 Z  2 160.0  $ Upper blanket
09 Z  2 180.0  $ Upper struct

14  C1P  PU239  0.0011   U238  0.0064
14  C1P  NA     0.0104   FE    0.0181    O-16  0.0149
14  C1   PU239  0.0011   U238  0.0064
14  C1   NA     0.0104   FE    0.0181    O-16  0.0149
14  C2   PU239  0.0015   U238  0.0054    NA    0.0110
14  C2   FE     0.0181   O-16  0.0138
14  AB   U238   0.0080   NA    0.0088    FE    0.0244
14  AB   O-16   0.0160
14  RB   U238   0.0145   NA    0.0066    FE    0.0173
14  RB   O-16   0.0290
14  RE   NA     0.0044   FE    0.0691
14  EMPTY1   NA     0.0220
14  EMPTY2   NA     0.0220
14  EMPTY3   NA     0.0220
14  EMPTY4   NA     0.0220
14  EMPTY5   NA     0.0220
14  NOROD1   NA     0.0220
14  NOROD2   NA     0.0220
14  NOROD3   NA     0.0220
14  NOROD4   NA     0.0220
14  NOROD5   NA     0.0220
14  ROD   NA     0.0104   FE    0.0181    O-16  0.0149
14  ROD   B-10   0.0090   C     0.0412

15    RE     REFL
15    AB     ABLAN
15    RB     RBLAN
15    C1     CORE1
15    C2     CORE2
15    EMPTY1 ROD1A
15    EMPTY2 ROD2A
15    EMPTY3 ROD3A
15    EMPTY4 ROD4A
15    EMPTY5 ROD5A
15    NOROD1 ROD1B
15    NOROD2 ROD2B
15    NOROD3 ROD3B
15    NOROD4 ROD4B
15    NOROD5 ROD5B

29  9.5
30  REFL    1   0  0  0.0 180.0
30  REFL    2   0  0  0.0 180.0
30  REFL    3   0  0  0.0 180.0
30  REFL    4   0  0  0.0 180.0
30  REFL    5   0  0  0.0 180.0
30  REFL    6   0  0  0.0 180.0
30  REFL    7   0  0  0.0 180.0
30  REFL    8   0  0  0.0 180.0
30  REFL    9   0  0  0.0 180.0
30  REFL   10   0  0  0.0 180.0

30  ABLAN    1   0  0 20.0 160.0
30  ABLAN    2   0  0 20.0 160.0
30  ABLAN    3   0  0 20.0 160.0
30  ABLAN    4   0  0 20.0 160.0
30  ABLAN    5   0  0 20.0 160.0
30  ABLAN    6   0  0 20.0 160.0
30  RBLAN    7   0  0 20.0 160.0
30  RBLAN    8   0  0 20.0 160.0

30  CORE1   1   0  0 40.0 140.0
30  CORE1   2   0  0 40.0 140.0
30  CORE1   3   0  0 40.0 140.0
30  CORE2   4   0  0 40.0 140.0
30  CORE2   5   0  0 40.0 140.0
30  CORE2   6   0  0 40.0 140.0

30   ROD1A   1   0  0 0.0  120.0
30  ROD2A    4   1  1 0.0  100.0
30  ROD3A    4   4  4 0.0   90.0
30  ROD2A    4   7  7 0.0  110.0
30  ROD3A    4  10 10 0.0  120.0
30  ROD2A    4  13 13 0.0   70.0
30  ROD3A    4  16 16 0.0   60.0
30   ROD4A   6   1  1 0.0   50.0
30   ROD5A   6   6  6 0.0  130.0
30   ROD4A   6  11 11 0.0  140.0
30   ROD5A   6  16 16 0.0  150.0
30   ROD4A   6  21 21 0.0  160.0
30   ROD5A   6  26 26 0.0  170.0

30   ROD1B   1   0  0 120.0 180.0
30  ROD2B    4   1  1 100.0 180.0
30  ROD3B    4   4  4  90.0 180.0
30  ROD2B    4   7  7 110.0 180.0
30  ROD3B    4  10 10 120.0 180.0
30  ROD2B    4  13 13  70.0 180.0
30  ROD3B    4  16 16  60.0 180.0
30   ROD4B   6   1  1  50.0 180.0
30   ROD5B   6   6  6 130.0 180.0
30   ROD4B   6  11 11 140.0 180.0
30   ROD5B   6  16 16 150.0 180.0
30   ROD4B   6  21 21 160.0 180.0
30   ROD5B   6  26 26 170.0 180.0
…
```

Figure 2-3. The DIF3D A.NIP3 Input Excerpt for the DIF3D Consistency Check

2.1.1 *Null Perturbation Test Case*

The first verification task is to ensure that the base DIF3D calculation that PERSENT initiates matches the provided DIF3D input with the input constraints applied to it by PERSENT. In this regard, the PERSENT manual [1] indicates that its primary focus is on modifying the user input in A.DIF3D and A.HMG4C that controls the type of problem being solved by DIF3D and the approximations used. For the present testing, PERSENT should not alter the geometry or cross sections unless directed to do so by the perturbation input. In the standard perturbation approach, the adjoint flux solution for the base state is needed while the forward flux solution is needed for the perturbed state. The reference solutions for both states will be obtained by manual manipulation of the DIF3D input. With the control rod setup described earlier, a null perturbation can be introduced as done in Figure 2-4 where a zone name is changed by PERSENT but it has no impact as the two zones were defined identically in Figure 2-3.

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   ./dif3d.x
DIF3D_INPUT        ./dif3d_a.inp
ADJUST_ZONE       TEST GENERALIZED_PT NOROD1 NOROD2
```

Figure 2-4. The PERSENT Null Perturbation Input for the DIF3D Consistency Check

In Figure 2-4, the PERSENT input is very simple where the FORCE_FULL_FLUX flag (FFF) is the key focus of the current verification work. The next three lines of input in Figure 2-4 specify the location of the dif3d executable and the base DIF3D input to work with. The last input specifies a perturbation where zone NOROD1 is replaced with zone NOROD2. As stated, these two zones have identical compositions, as shown in Figure 2-3, and this is a null perturbation with a zero worth. The DIF3D control input that PERSENT modifies is in A.DIF3D and A.HMG4C, and example DIF3D inputs are provided in Figure 2-5.

```
UNFORM=A.DIF3D
01       Some problem to run
02    999999  20000000
03    0 2 0 0 300 0 0 1 0 0
04    1 1 1 11 111 11 111 1 1 0001
05            1.0E-8    1.0E-7       1.0E-7
06    1.0 1.0E-4 0.04 333.333E+6
12    472 11 -1 0 0 -1 1   0 0
UNFORM=A.HMG4C
02   1E8 0 0 0 0 1
```

Diffusion

```
UNFORM=A.DIF3D
01       Some problem to run
02    999999  20000000
03    0 2 0 0 300 0 0 1 0 0
04    1 1 1 11 111 11 111 1 1 0001
05            1.0E-8    1.0E-7       1.0E-7
06    1.0 1.0E-4 0.04 333.333E+6
12    40601 33 -1 0 0 -1 1   1 1
UNFORM=A.HMG4C
02   1E8 0 0 0 0 0
```

Transport

Figure 2-5. Example Diffusion and Transport DIF3D Input for the DIF3D Consistency Check

The important inputs that PERSENT will modify are colored red in Figure 2-5. For card type 03, the second input allows the user to select whether to run the forward, adjoint, or both flux solutions. PERSENT will also modify other values on this card input for sensitivity calculations but those will be verified later during the sensitivity verification work. Card type 12 is used to specify the VARIANT space-angle approximations of the flux and current along with other controls. The first number on card type 12, 472 in the diffusion example, indicates the spatial polynomial approximation to be used by VARIANT for the source, flux, and currents. DIF3D will take this input and modify it to become 040722 as outlined in the DIF3D-VARIANT manual [9]. In the PERSENT manual [1], PERSENT will modify this user input to 70722 if the user specifies the flag “FORCE_FULL_FLUX” (FFF) is enabled. The second input on card type 12, 11 in the diffusion example, indicates the angular approximation to be used by VARIANT for the flux and currents. As stated in the PERSENT manual, PERSENT will modify this input to 10101 if the user specifies the FFF flag.

The 6th number on card type 12, -1 in both examples, is used to enable or disable the 30 degree and 45 degree symmetry options of VARIANT. If the hex geometry provided by the user has 30 degree symmetry, VARIANT will only solve the hexes that appear in the lower 30 degree sector and copy the flux solution into the upper hexes. Because PERSENT uses the flux solution with the operator, the flux solution copied from the lower hexes should also be rotated internally to DIF3D when they are copied to the upper hexes. Since modifying DIF3D to do this was not desired in the PERSENT development, PERSENT simply prevents the user from using the 30 or 45 degree symmetry option to avoid producing incorrect results. The 30 degree symmetry only applies when the user provides a 60 degree periodic geometry while the Cartesian 45 degree symmetry option only applies when the –X and –Y boundary conditions are reflective and the meshing in X and Y are identical. Neither of these options are routinely used today for reactor analysis.

The 8th and 9th numbers on card type 12 control the anisotropic scattering kernel. PERSENT requires these numbers to be identical to prevent problems with the anisotropic scattering kernel re-normalization internal to DIF3D. Given the methodology to produce the scattering kernel in MC^2 was not built to be consistent with the renormalization methodology in DIF3D-VARIANT, this feature was not propagated into PERSENT and thus PERSENT disables it. From the PERSENT manual, if the FFF flag is provided, PERSENT will also modify the 8th and 9th inputs, along with the provided ISOTXS data, to force DIF3D-VARIANT to reconstruct the full angular expansion used for the flux.

The last section of input that PERSENT will modify is in A.HMG4C. Figure 2-5 shows two examples for diffusion and transport. As indicated, only the 6th number on card type 02 is modified by PERSENT. This input has to do with the isotopic based fission emission spectrum data. PERSENT will force this value to be a 1 as this is again consistent with the way that MC^2 is producing data. As will was discussed in the PERSENT manual [1], PERSENT allows the user to generate the NHFLUX and NAFLUX files on their own. It is entirely possible for the user to generate those flux files without using the isotopic based fission emission spectrum and thus PERSENT will have an inconsistency in the operator it is using versus the provided flux files and thus produce erroneous perturbation and sensitivity results. This aspect of verification is not covered in this report as the PERSENT manual makes it very clear that the user should allow PERSENT to generate the proper input for a given perturbation or sensitivity problem.

The set of tests to perform are shown in Table 2-1. Each row of this table provides the DIF3D inputs that are used to define the base state. For each DIF3D case, the forward and adjoint eigenvalues are requested via the input and thus the two eigenvalues in each cell of the table provide the adjoint eigenvalue first (upper one) followed by the forward eigenvalue (lower one). For PERSENT, the first eigenvalue is for the adjoint solution of the base state while the second is the forward solution of the perturbed state. Since the perturbation is a null perturbation, there should be negligible differences between the two forward eigenvalues. The DIF3D input and reference output for this test case are distributed as benchmark 42 in the DIF3D distribution. The PERSENT input and reference output for this test case correspond to benchmark 20 in the PERSENT distribution.

Table 2-1. Null Perturbation Eigenvalue Results for the DIF3D Consistency Check.

Test #	VARIANT Input			DIF3D		PERSENT	
	Space	Angle & Scat. Kernel	Isotopic Fission Spec.	Base	Manually Modified Input	Option #1 No Force Full Flux	Option #2 Force Full Flux
1	20721	P_1 P_0	Yes	0.89452 791 0.89452 776	0.89454 042 0.89454 028	0.89452 791 0.89452 779	0.89454 043 0.89454 025
2	20701	P_3 P_1	Yes	0.94702 218 0.94702 212	0.94703 933 0.94703 926	0.94702 220 0.94702 214	0.94703 931 0.94703 925
3	20701	P_1 P_0	**No**	0.89460 853 0.89460 839	0.89454 051 0.89454 037	0.89452 803 0.89452 785	0.89454 049 0.89454 037

The first test (Test #1) in Table 2-1 is for a full core hexagonal geometry model and corresponds to the a and b labeled files in the verification test distribution. The DIF3D adjoint and forward eigenvalues for the base state are within 0.015 pcm of each other which indicates some amount of iterative error remains as the eigenvalues should be identical. When the FFF flag is set, the spatial approximation should be modified by PERSENT from 20721 to 70721. The manually modified input for this alteration (sixth column in table), indicates a 1.3 pcm change in the eigenvalue when the input change is made (fifth to six column in table). The PERSENT reported eigenvalues also yield a 1.3 pcm change (seventh to eight column in table).

Looking at the PERSENT reported eigenvalues, one finds they are very similar to the DIF3D calculated ones but have errors in the last significant digit (maximum 0.003 pcm error). The error has to do with truncation of the DIF3D result when it is stored in the NHFLUX binary interface file (stored as 32 bit real instead of 64 bit real) [8,10]. This aspect will lead to differences on this magnitude seen here even if 10^{-10} is used for the eigenvalue convergence. This does not indicate a defect in PERSENT, but a simple limitation on the calculable perturbation worth in PERSENT to $>10^{-8}$ because of the 32 bit truncation of the solution data.

The second test in Table 2-1 uses transport with the 60 degree periodic geometry option of DIF3D and corresponds to c and d labeled files in the verification test distribution. Because the base configuration was setup to be radially symmetric, the 60 degree periodic geometry result is equivalent to the full core geometry result. The differences in the eigenvalues between the first and second test cases are entirely due to using diffusion theory versus transport theory and they are consistent with past experience. With regard to the iterative convergence, both DIF3D and PERSENT show errors of ~0.007 pcm between the forward and adjoint eigenvalues. The DIF3D and PERSENT reported eigenvalues differ by less than 0.002 pcm. Finally, using the 20701 setting versus 70701 is found to be ~1.71 pcm by both DIF3D and PERSENT.

The third test in Table 2-1 uses diffusion theory with a 120 degree periodic geometry and corresponds to e and f labeled files in the verification test distribution. While the spatial approximation is again manipulated by PERSENT, the isotopic fission flag in A.HMG4C is the real point of this test. In Table 2-1, the base DIF3D eigenvalues are within 0.014 pcm of each other indicating the amount of residual iterative convergence left. The manual modification of the DIF3D input produces a -6.8 pcm change in the eigenvalue and the slight difference in the spatial approximation (20721 versus 20701) should make it clear that the isotopic fission flag is responsible for a bulk of the change in the eigenvalue. As seen, the option 1 approach of running PERSENT will produce eigenvalues in strong disagreement with the base DIF3D results. As

stated, PERSENT will engage the isotropic fission flag for ANY provided input and thus different answers with respect to DIF3D are possible.

From Table 2-1, the test 1 and test 3 eigenvalue results for DIF3D (column 5 results) are not the same while the test 1 and test 3 eigenvalue results (column 7 and 8) for PERSENT are nearly identical. It should be clear that PERSENT is imposing the isotropic fission flag when using option 1 or option 2. Additional DIF3D calculations to verify that this is the source of the discrepancy were done but not documented here. The manually modified DIF3D input exactly matches the second PERSENT option indicating again that the behavior of PERSENT with the FFF flag and isotopic fission flag adjustment are working as expected.

Looking at the PERSENT reported eigenvalues in Table 2-1, it should be clear that without the FFF flag, PERSENT does not make changes to the user input and the two eigenvalues are nearly identical to the base DIF3D ones (columns 5 and 7 match along with 6 and 8 for test #1 and #2). The expected behavior of the FFF flag for option 2 of PERSENT is to increase the source order to be consistent with the flux (20701 to 70701 or 20721 to 70721). It will also modify the anisotropic scattering kernel to P_3 where any P_2 or P_3 data present would be zeroed out by PERSENT. The verification test problems provided with PERSENT and documented in the manual are sufficient to verify that the ISOTXS modification occurs properly and that aspect is not checked as part of this test problem (this cross section set only has P_1 scattering data). Figure 2-6 shows the PERSENT output for the first option of the first test case in Table 2-1. The last line provides the total computed worth which is zero which was expected as the perturbation did not actually change the model. All of the other test cases and FFF options also report zero worths from the null perturbation as expected. The eigenvalues shown in Figure 2-6 are those that appear in Table 2-1 above for test #1 option #1.

```
…
[PERSENT]...Warning, could not find default ISOTXS file: ./user.ISOTXS
[PERSENT]...Creating the modified DIF3D input deck
[PERSENT]...Running a null DIF3D job to create the input
[PERSENT].................................................
[PERSENT]...Entering main branch of the PERSENT code.......
[PERSENT].................................................
[PERSENT]...Processing the ISOTXS file
[PERSENT]...Checking the user input materials
[PERSENT]...Checking the PERSENT materials data
[PERSENT]...Checking the PERSENT input data for the perturbation options
[PERSENT]...Checking the PERSENT input data for the sensitivity options
[PERSENT]...Running a null DIF3D job to create the forward COMPXS file
[PERSENT]...Running DIF3D to get the unperturbed adjoint solution
[PERSENT]...Carrying out all perturbation input problems
[PERSENT]..........................................................................
[PERSENT]...Problem TEST             is a zone perturbation using GENERALIZED_PT
[PERSENT]...Associated DIF3D output is P_dif3d_problem0001.out
[PERSENT]..........................................................................
[PERSENT]...Replacing zone     NOROD1   with copy of zone     NOROD2
[PERSENT]...Running DIF3D to get the perturbed forward solution
[PERSENT]...Performing the DIF3D-VARIANT numerator/denominator operations
=PERSENT...Parameter General PT of TEST   is  0.00000E+00 denominator  4.92474E+29 k-eff A  8.9452791E-01 F  8.9452779E-01
```

Figure 2-6. The PERSENT Output Excerpt for the Null Perturbation DIF3D Consistency Check

Figure 2-7 provides an excerpt of the DIF3D input that PERSENT generates when running DIF3D for option #2 of the transport test case (test #2). The card type 12 inputs are highlighted and indicate that PERSENT has modified those inputs consistently with that stated in the manual. Inspection of the flux and power tables from DIF3D indicates that the DIF3D calculated results were identical but is not documented here for brevity. Combined, these three tests confirm the

interpretation of how PERSENT will modify the user input, as described in the manual and detailed above.

```
…
  BLOCK=OLD
  DATASET=ISOTXS
  DATASET=NDXSRF
  DATASET=ZNATDN
  DATASET=GEODST
  DATASET=LABELS
  BLOCK=STP021,3
  UNFORM=A.DIF3D
   1       Some problem to run
   2      20000000   20000000  0
   3     0 1 0  10000   1000 0 1000000000    1    0    0   50
   4         0     0     0     0     0     0     0     0     0     1
   5           1.00000E-08 1.00000E-07 1.00000E-07
   6   1.00000000E+00  1.00000E-04  4.00000E-02  3.33333E+08  0.00000E+00
  12     70701 10303    -1     0     0    -1     1     3     3     0     0
  12         1     0     0
  UNFORM=A.HMG4C
  01    PERSENT DISABLES HMG4C EDITS
  02  20000000   1     0     0     0     1
…
```

Figure 2-7. Null Perturbation Input Excerpt for the Second DIF3D Consistency Check

2.1.2 *Control Rod Perturbation Tests*

In this verification test, the control rod material will be used to create a perturbation and the PERSENT results will be verified by manual manipulation of the provided DIF3D input. The DIF3D inputs are included as benchmark 43 in the DIF3D distribution while the PERSENT verification test problems are included as benchmark 21 in the PERSENT distribution. The total perturbation worth will be compared with the exact value and the region-wise distribution of the control rod worth produced by PERSENT will be checked. The mesh-wise perturbation will be checked in a later section as the hand calculation of the mesh-wise values is cumbersome. As discussed earlier, the base DIF3D input has 5 control rod regions and Figure 2-8 shows the PERSENT input excerpt indicating that 7 control rod perturbations are carried out. In the first perturbation (named TEST1), control rod 1, 2, and 5 (NOROD1, NOROD2, NOROD5) are perturbed to replace the empty control rod material with the rodded one. For the second perturbation (TEST2), all five control rods are perturbed in the same manner. In the remaining 5 perturbations (TEST3 to TEST7), each control rod region is perturbed individually. All of these perturbations have to be carried out using a full core hexagonal geometry model option.

```
…
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD1 ROD
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD2 ROD
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD5 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD1 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD2 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD3 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD4 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD5 ROD
ADJUST_ZONE      TEST3 GENERALIZED_PT NOROD1 ROD
ADJUST_ZONE      TEST4 GENERALIZED_PT NOROD2 ROD
ADJUST_ZONE      TEST5 GENERALIZED_PT NOROD3 ROD
ADJUST_ZONE      TEST6 GENERALIZED_PT NOROD4 ROD
ADJUST_ZONE      TEST7 GENERALIZED_PT NOROD5 ROD
…
```

Figure 2-8. The PERSENT Control Rod Perturbation Input for the DIF3D Consistency Check

Because the FFF flag has already been tested and verified, the DIF3D inputs were made to be identical to what PERSENT will generate (the isotopic fission spectrum flag is engaged). To

reduce the computational expense associated with the verification process, a flat spatial leakage approximation is used in DIF3D-VARIANT. The DIF3D and PERSENT reported eigenvalues for the base state and the seven perturbations are provided in Table 2-2. The two values reported for the base DIF3D state are for the adjoint (upper) and forward (lower) flux solutions. As can be seen, the forward and adjoint eigenvalues have a 0.056 pcm error in the diffusion case and 0.010 pcm error in the transport calculation. Both of these are due to the residual iterative error in the system. The reported adjoint eigenvalue from PERSENT on the base state is identical to the adjoint eigenvalue obtained in the DIF3D calculation. For all of the perturbation calculations, only the forward eigenvalue solution was obtained from DIF3D for the diffusion and transport calculations to be consistent with what PERSENT is doing.

Table 2-2. Control Rod Perturbation Results for the DIF3D Consistency Check.

	Diffusion		Transport			
	DIF3D	PERSENT	DIF3D	PERSENT	Worth (pcm)	
Base	0.89572 175 0.89572 232	0.89572 173	0.95337 449 0.95337 439	0.95337 451	DIF3D	PERSENT
1	0.86677 586	0.86677 587	0.92345 374	0.92345 375	-3399	-3399
2	0.83918 483	0.83918 482	0.89496 810	0.89496 809	-6845	-6845
3	0.89190 880	0.89190 882	0.94947 127	0.94947 129	-431.2	-431.2
4	0.86969 888	0.86969 888	0.92645 159	0.92645 156	-3048	-3048
5	0.86692 583	0.86692 584	0.92352 922	0.92352 921	-3390	-3390
6	0.89189 951	0.89189 953	0.94933 180	0.94933 182	-446.7	-446.7
7	0.89549 349	0.89549 351	0.95309 834	0.95309 836	-30.38	-30.38

In Table 2-2, the perturbation worth for the transport case is hand calculated using the DIF3D results with the equation

$$\rho = \frac{1}{k_{base}} - \frac{1}{k_{perturbed}}. \quad (1)$$

The PERSENT output excerpt that reports the perturbation worth of each problem is given in Figure 2-9. The results for both the hand calculated DIF3D and PERSENT are provided in Table 2-2 and are identical. It should be noted that the slight differences in the eigenvalues do not appear in the perturbation worth as more significant digits on the output are required. As seen from the PERSENT output excerpt, the DIF3D reported eigenvalues in Table 2-2 are slightly different (maximum 0.003 pcm error) from those reported by PERSENT which is again the round off error that comes from storing and retrieving the values from the binary NHFLUX interface file. The power and flux details printed as part of the regular DIF3D output were compared for the manual manipulation and the PERSENT directed outputs. No differences were found in the spatial distribution of flux or power in that work and it is not shown here for brevity.

```
…
=PERSENT...Parameter General PT of TEST1 is -3.39852E-02 denominator  5.58781E+29 k-eff A  9.5337451E-01 F  9.2345375E-01
=PERSENT...Parameter General PT of TEST2 is -6.84519E-02 denominator  5.59401E+29 k-eff A  9.5337451E-01 F  8.9496809E-01
=PERSENT...Parameter General PT of TEST3 is -4.31185E-03 denominator  5.58123E+29 k-eff A  9.5337451E-01 F  9.4947129E-01
=PERSENT...Parameter General PT of TEST4 is -3.04812E-02 denominator  5.58344E+29 k-eff A  9.5337451E-01 F  9.2645156E-01
=PERSENT...Parameter General PT of TEST5 is -3.38967E-02 denominator  5.57940E+29 k-eff A  9.5337451E-01 F  9.2352921E-01
=PERSENT...Parameter General PT of TEST6 is -4.46659E-03 denominator  5.58658E+29 k-eff A  9.5337451E-01 F  9.4933182E-01
=PERSENT...Parameter General PT of TEST7 is -3.03800E-04 denominator  5.57879E+29 k-eff A  9.5337451E-01 F  9.5309836E-01
…
```

Figure 2-9. The PERSENT Control Rod Worth Excerpt for the DIF3D Consistency Check

2.1.3 *Summary of the DIF3D Consistency Check*

In the preceding examples, the PERSENT capability of modifying the user input to DIF3D was demonstrated. For all cases with the FFF flag enabled, PERSENT exactly matched the manually modified DIF3D results. Both the DIF3D outputs produced via PERSENT and the PERSENT computed worth matched the exact perturbation result. Without the FFF flag enabled, PERSENT produced the correct total worth.

Additional verification of the PERSENT modifications to the user input will be done as part of the sensitivity verification work. The preceding verification is comprehensive for the perturbation theory options and thus no further work needs to be done to satisfy Category 1 of Table 1-1.

2.2 Exact Perturbation Verification

Category 2 from Table 1-1 is focused on the accuracy of the exact perturbation theory option of PERSENT. Task a of category 2 is intended to confirm that the DIF3D solution generated by PERSENT is correct. In the previous section, two example perturbation cases were provided for the zone perturbation input option of PERSENT (ADJUST_ZONE) and do not need to be completed again. This leaves the four other input options to be checked: ADJUST_XS, ADJUST_DENSITY, ADJUST_GENERIC, and BOWING_WORTH. Task b is focused on the spatial distribution of worth which, as will be shown, is very difficult to demonstrate for non-trivial test cases. Task c and d are focused on the mass change calculation available in the perturbation theory ADJUST_ZONE input and the alternative representation of the worth. This input is specifically generated by PERSENT to provide direct input to SAS4A.

2.2.1 *Verification of the DIF3D Accuracy in Exact Perturbation Calculations*

For ADJUST_XS, ADJUST_DENSITY, and ADJUST_GENERIC, the verification process is identical to that done for ADJUST_ZONE in the previous section. Because the BOWING_WORTH approach is based upon the first order perturbation methodology, it will not be covered in this section as the perturbed state eigenvalue is not computed by PERSENT. The same base input defined by Figure 2-1 is used in this test work. Both diffusion and transport options are tested and the PERSENT specific input for this series of tests is given in Figure 2-10. The DIF3D test cases discussed here are benchmark 44 in the DIF3D distribution while the PERSENT test cases are benchmark 22 in the PERSENT distribution.

In Figure 2-10, the ISOTOPE_LIST input option is used to select specific isotopes (PU239 and FE) from ISOTXS. For consistency, an example of the ADJUST_ZONE input is provided as TEST1 where zone NOROD1 is to be replaced with zone ROD. TEST2 and TEST3 are both density adjustments. For TEST2, the density of zone EMPTY1 is modified by a factor of 2.0 while for TEST3 the density of zone C1 is modified by a factor of 1.3. TEST4 and TEST5 are both cross section perturbations. In TEST4, the fission cross section of isotope PU239 is modified by a factor of 0.5 in group 1. In TEST5, the elastic scattering cross section of FE is increased by 0.1 for groups 1 through 3 (the entire matrix is adjusted by this amount).

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   ./dif3d.x
DIF3D_INPUT        ./dif3d_a.inp

ISOTOPE_LIST PU239 PU239
ISOTOPE_LIST IRON  FE

ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD1 ROD
ADJUST_DENSITY   TEST2 GENERALIZED_PT EMPTY1 2.0
ADJUST_DENSITY   TEST3 GENERALIZED_PT C1     1.3
ADJUST_XS        TEST4 GENERALIZED_PT PU239 fission 0.5 0.0 1 1
ADJUST_XS        TEST5 GENERALIZED_PT IRON  elastic 1.0 0.1 1 3
ADJUST_GENERIC   TEST6 GENERALIZED_PT dif3d_ap3.inp
ADJUST_GENERIC   TEST7 GENERALIZED_PT dif3d_ap7.inp
ADJUST_GENERIC   TEST7 GENERALIZED_PT dif3d_ap8.inp

PROBLEM_EDITS    TEST1 PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
PROBLEM_EDITS    TEST2 PRINT_BY_REGION PRINT_BY_MESH PRINT_BY_MASS PRINT_BALANCE
PROBLEM_EDITS    TEST3 PRINT_BY_REGION PRINT_BY_MESH PRINT_BY_MASS PRINT_BALANCE
PROBLEM_EDITS    TEST4 PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
PROBLEM_EDITS    TEST5 PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
PROBLEM_EDITS    TEST6 PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
PROBLEM_EDITS    TEST7 PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
PROBLEM_EDITS    TEST8 PRINT BY REGION PRINT BY MESH PRINT BALANCE
```

Figure 2-10. The PERSENT Input for DIF3D Perturbation Theory Check

The last three tests use the ADJUST_GENERIC feature of PERSENT. In the ADJUST_GENERIC methodology, the user just provides a modified DIF3D input that specifies the perturbation noting that the number of spatial meshes cannot change. TEST6 repeats TEST3 (dif3d_ap3.inp) test. TEST7 and TEST8 modify the C1 composition and adjust the assembly pitch as shown in Figure 2-11. Referring to Figure 2-3, the original C1 composition is broken into sodium and the other isotopes. The new C1 composition in both TEST7 and TEST8 keeps the same sodium density but reduces the other isotopic densities by a factor of 0.99. For TEST7, the assembly pitch is increased from 9.5 cm to 9.75 cm where in TEST8 it is kept at 9.5 cm.

```
14  C1aa   PU239  0.0011   U238  0.0064
14  C1aa   FE    0.0181    O-16  0.0149
14  C1bb NA     0.0104
14  C1MOD C1aa 0.99 C1bb 1.0
15    C1MOD  CORE1
29  9.75
```

TEST7

```
14  C1aa   PU239  0.0011   U238  0.0064
14  C1aa   FE    0.0181    O-16  0.0149
14  C1bb NA     0.0104
14  C1MOD C1aa 0.99 C1bb 1.0
15    C1MOD  CORE1
29  9.5
```

TEST8

Figure 2-11. ADJUST_GENERIC Specific DIF3D Input Modifications

The eigenvalue results for the DIF3D (manual modification of the input) and PERSENT and the computed worth are provided in Table 2-3 for diffusion theory and Table 2-4 for transport. The diffusion problem used a 2^{nd} order flux and source and a 0^{th} order current approximation while the transport problem used a 6^{th} order flux and source, a 1^{st} order leakage, a P_3 angular flux, and P_1 scattering kernel approximations. The transport settings are the standard ones in use today.

Table 2-3. Perturbation Theory Eigenvalue Results for Diffusion.

	DIF3D	PERSENT	Worth (pcm)			80803	
	0.89572 175 0.89572 232	0.89572 173	DIF3D	PERSENT	Error	Error	%
TEST1	0.89190 880	0.89190 882	-477.3	-477.3	0.06	-0.02	0.003
TEST2	0.89609 338	0.89609 337	46.30	46.22	0.08	-0.02	-0.051
TEST3	0.92499 435	0.92499 435	3533.0	3532.3	0.73	0.65	0.018
TEST4	0.84142 334	0.84142 333	-7204.4	-7204.5	0.07	-0.01	0.000
TEST5	0.92457 916	0.92457 914	3484.5	3484.4	0.10	0.01	0.000
TEST6	*0.92499 435*	0.92499 435	3533.0	3532.3	0.73	0.65	0.018
TEST7	0.90412 072	0.90412 074	1037.1	1036.7	0.44	0.35	0.034
TEST8	0.89470 247	0.89470 249	-127.2	-127.2	0.05	-0.04	0.030

Table 2-4. Perturbation Theory Eigenvalue Results for Transport.

	DIF3D	PERSENT	Worth (pcm)			80803	
	0.95337449 0.95337439	0.95337 451	DIF3D	PERSENT	Error	Error	%
TEST1	0.94947 127	0.94947 129	-431.2	-431.2	-0.01	-0.01	0.005
TEST2	0.95323 833	0.95323 831	-14.98	-14.97	-0.02	-0.02	0.181
TEST3	0.97972 445	0.97972 447	2821.1	2820.4	0.62	0.62	0.021
TEST4	0.89625 298	0.89625 299	-6685.1	-6685.1	-0.01	-0.02	0.000
TEST5	0.98181 211	0.98181 212	3038.1	3038.1	0.01	0.02	0.000
TEST6	*0.97972 445*	0.97972 447	2821.1	2820.5	0.61	0.62	0.021
TEST7	0.96138 006	0.96138 006	873.4	873.1	0.32	0.33	0.036
TEST8	0.95243 008	0.95243 007	-104.0	-104.0	-0.03	-0.03	0.036

For comparison, the spatial approximation was increased to an 8th order flux and source approximation and the leakage to 3rd order (80803) to verify that these are not contributing issues and the results are included in both tables as the two right hand most columns. It is important to note that the TEST6 problem is identical to TEST3 and thus the eigenvalue result is just duplicated for DIF3D.

A quick comparison of the DIF3D and PERSENT reported eigenvalues shows a near identical match in both diffusion and transport for all of the test cases where the differences are again due to the NHFLUX file truncation of the eigenvalue. A review of the worth results show that all of the PERSENT computed worths have errors with respect to the DIF3D computed results for all of the test cases. The error typically occurs in the 4th or 5th significant digit of the total worth and the largest magnitude errors occur with TEST3, TEST6, and TEST7 but the largest percentage error occurs with TEST2. TEST2 and TEST3 are very similar and involve a simple density change while TEST3 and TEST6 are the same problem ran with two different perturbation options in PERSENT. TEST7 is the ADJUST_GENERIC case with a geometric pitch change.

This residual error issue is discussed in section 2.7 and section 6.3 of the PERSENT manual and applies to TEST7 and TEST8. In the manual, it states that this error is due to the lack of beneficial cancellation of error in the operator application when the geometric pitch is modified. In the testing shown here, both TEST7 and TEST8 exhibit a similar magnitude of error, ~0.03% of the total worth, and the manual clearly indicates that this is not unusual. Similar statements are made about the other perturbation options in section 6.2 of the PERSENT manual and attribute the issue to lack of iterative convergence. Tightening the iterative convergence on all of the test cases in Table 2-3 and Table 2-4 made little difference in the actual error between PERSENT and the

direct DIF3D eigenvalue. Because the magnitude of the error is random and not consistent with the magnitude of the perturbation being applied, it is fair to say that:

1) the magnitude of the error observed is negligible with respect to the total worth

2) the error is likely due to some other aspect from what the developers state in the manual

With regard to the latter, potential sources include some other dependence on single precision values in the interface files that have not been identified or an inconsistency in the operator being applied in PERSENT versus the one in DIF3D that may again involve single precision versus double precision intermediate values in DIF3D. In any case, the computed results from PERSENT on these tests are very consistent with the exact computed result from DIF3D for a wide range of perturbation magnitudes and the observed errors are simply not large enough, nor consistent enough, to be of concern.

The preceding test cases are sufficient to demonstrate that all perturbation options of PERSENT are working as expected. There is no clear reason for the residual error between the eigenvalue computed result and the one being obtained with the operator in PERSENT at this time, but its observed magnitude is relatively unimportant. There is no way to guarantee that the observed error in the worth will remain small without understanding the issue. Since the PERSENT software has been around for a while, and no identified issues have been presented by the developers, it is unlikely that the magnitude of the observed error is actually important for any follow-on analysis capability.

2.2.2 *Manual Calculations of the Mesh-wise Perturbation Worth*

The mesh- and region-wise perturbation results from PERSENT can be onerous to verify. In the earlier control rod worth tests, all of the PERSENT perturbation outputs were verified but only one is selected here to display the difficulty in verifying the mesh-wise PERSENT result. TEST3 from Figure 2-8 was chosen as it involves a single hexagonal position and only six meshes. The PERSENT output excerpt for this test problem is displayed in Figure 2-12. The DIF3D test cases discussed here are benchmark 45 in the DIF3D distribution while the PERSENT test cases are benchmark 23 in the PERSENT distribution.

Because the control rod only occurs at a single radial position, the reactivity worth spatial distribution only has a single non-zero value per plane for those axial planes which have a perturbation. The first section of output shows a sub-set of the 13th radial plane of results for this perturbation with the only non-zero value being -2.543E-03 at position 10,10. The full radial map has 19 rows and 19 columns of hexagon data. For full core models in DIF3D-VARIANT, one can compute the number of rows (and columns) in this output by subtracting one from the number of rings multiplied by 2 (e.g. 10*2-1=19). The input from Figure 2-3 can be used to confirm that there are 10 rings of input provided to DIF3D. The center position in the 19x19 matrix of values should occur at row 10 and column 10. The only non-zero output in Figure 2-12 occurs exactly at position 10,10 for all axial planes and the control rod position in Figure 2-3 corresponds to the center hexagon of the domain thereby verifying that the location of the output is correct.

The next section of the PERSENT output in Figure 2-12 provides just the 10th row result for the axial planes 14 through 18. These correspond to each axial mesh in the input geometry from Figure 2-3 where the control rod was inserted. The last section of output in Figure 2-12 provides the region summary of the perturbation worth. Because the perturbation worth is stored mesh wise

internal to PERSENT, as is evident from the output, the constraints of only allowing zone-wise perturbations in the PERSENT input do not impact the region-wise perturbation output.

```
…
[PERSENT]...Axial plane     13 data for General PT of TEST3
                1           2           3           4           5           6           7           8           9          10
    19  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    18  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    17  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    16  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.543E-03
…
[PERSENT]...Axial plane     14 data for General PT of TEST3
…
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.197E-03
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -4.058E-04
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.285E-04
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -3.610E-05
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.192E-06
…
[PERSENT]...Region edits for General PT of TEST3
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|ABLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|RBLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD1A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD2A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD1B | -2.407E+27|        -4.312E-03|
[PERSENT]...|ROD2B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5B |  0.000E+00|         0.000E+00|
=PERSENT...Parameter General PT of TEST3 is -4.31185E-03 denominator  5.58123E+29 k-eff A  9.5337451E-01 F  9.4947129E-01
…
```

Figure 2-12. The PERSENT Output Excerpt for the 3rd Control Rod Perturbation

Summing the values in the spatial reactivity worth distribution in Figure 2-12 produces 4.3116E-3 which is within round-off error from the PERSENT reported region wise result of 4.312E-03. Both of these values are in turn within round-off error from the total worth of 4.31185E-03 reported by PERSENT. One can hand calculate the same number given the total region-wise numerator value and the domain-wise denominator values from Figure 2-12. For ROD1B this is -2.407E27/5.58123E29=-4.3127E-03. Again this result is within round-off error of the total worth. This verifies that the PERSENT output is self-consistent on both the mesh-wise and region-wise basis.

To complete the verification, one should provide evidence that the mesh-wise values are accurate noting that the total worth has already been demonstrated to be correct. To hand calculate these values, one must be able to evaluate the perturbation equation from the PERSENT manual [1] given as

$$\rho = \frac{\langle \psi^*, B(\hat{\lambda})\hat{\psi}\rangle - \langle \psi^*, \hat{B}(\hat{\lambda})\hat{\psi}\rangle}{\langle \psi^*, F\hat{\psi}\rangle} = \frac{\langle \psi^*, B(\hat{\lambda})\hat{\psi}\rangle}{\langle \psi^*, F\hat{\psi}\rangle}. \quad (2)$$

In this equation, ψ^* represents the adjoint flux solution of the base state, $\hat{\psi}$ represents the forward flux solution of the perturbed state, $B(\hat{\lambda})$represents the base transport operator evaluated with the perturbed state eigenvalue $\hat{\lambda}$, $\hat{B}(\hat{\lambda})$represents the perturbed transport operator evaluated with the perturbed state eigenvalue, and F represents the base state fission source operator. Because the

transport operator involves a spatial derivative to account for the leakage, an exact hand calculation of equation 2 is not easy. More of an issue is that VARIANT uses a high order space-angle basis all of which are used in the collapsing process of the perturbation equation. In the remainder of this section, various hand calculations will be demonstrated to be inadequate for computing the mesh-wise reactivity worth.

The first approximate way of calculating the perturbation worth is to manually apply the perturbation worth in DIF3D for each mesh and sum the results. This is known to be inaccurate as the perturbed state flux solution defined by the original perturbation includes the impact of all mesh-wise perturbations while the proposed approximation does not. As the magnitude of the original perturbation increases, the changes in the flux solution between the individual mesh perturbations will increase and the error in the total perturbation will increase. To demonstrate how accurate this approach can be, Table 2-5 provides the stated separated calculation with DIF3D and the PERSENT on the transport problem. From Table 2-5, each spatial mesh perturbation with DIF3D over predicts the worth with respect to the PERSENT reported results. The final total worth has an error of ~10%.

Using Cartesian geometry, it is possible to show that one can actually achieve accuracy with the direct approach shown here by imposing mesh refinement. If the radial and axial meshes can be made small enough to have at most a linear flux shape in each mesh, then the direct DIF3D calculation approach should very nearly reproduce the PERSENT worth. Because it is not possible to sub-divide the hexagonal mesh in DIF3D-VARIANT, this approach is not an option and one can only hope that the results get close enough with finer meshing.

Table 2-5. Control Rod Mesh-wise Perturbation Results for the DIF3D Consistency Check.

Axial Mesh	DIF3D k_{eff}	DIF3D Worth (pcm)	PERSENT worth (pcm)
13	0.95089 726	-273.2	-254.30
14	0.95212 722	-137.4	-119.70
15	0.95295 344	-46.33	-40.58
16	0.95324 391	-14.36	-12.85
17	0.95333 949	-3.840	-3.610
18	0.95337 661	0.2442	-0.1192
		-474.93	-431.19

The axial meshing chosen for this test problem was 10 cm which is already rather fine for DIF3D-VARIANT where the typical limit is ~0.85 cm for sodium cooled fast spectrum reactors with regard to being able to get a converged solution. Because this control rod position was centrally located and the flux solution is radially rather symmetric, it is reasonable to assume that the radial shape of the forward and adjoint flux shape will cancel out when applied with the transport operator in the perturbation equation and thus one can investigate the direct mesh-wise perturbation approach in DIF3D but this was not done as this will not be the case for all perturbation problems of interest for PERSENT.

A second approach to computing the worth is to make use of the DIF3D balance edits. Returning to the perturbation equation, the numerator involves a sum over all regions of each

operator. Because the transport operators are both evaluated with the perturbed state eigenvalue and perturbed state flux, the only non-zero components of this operation will occur for those meshes with actual cross section perturbations. Thus one way to calculate the worth is to use the balance edits of DIF3D to evaluate the operator in the base and perturbed states. Figure 2-13 shows an example of the balance edits for the base state of the transport calculation.

```
…
DIF3D   11.3159 11/06/20            Some problem to run                                                    PAGE     22
REGION AND AREA BALANCE INTEGRALS FOR   REAL  K-EFF  PROBLEM WITH ENERGY RANGE (EV) =(8.006E+05,1.000E+07)  FOR GROUP    1
 REGION      ZONE  ZONE         NET    +  ABSORPTION +    SCATTER  -    SCATTER  -    FISSION  -    EXTERNAL =     BALANCE
NO.  NAME     NO.  NAME       LEAKAGE       RATE(1)        OUT(2)          IN       PRODUCTION(3)    SOURCE
  1  REFL       6  RE      -3.35154E+17   5.52521E+15   3.29629E+17   0.00000E+00   0.00000E+00   0.00000E+00  -1.55280E+09
  1  REFL       6  RE      -3.35154E+17   5.52521E+15   3.29629E+17   0.00000E+00   0.00000E+00   0.00000E+00  -5.41894E+06
  2  ABLAN      4  AB      -7.75315E+17   8.94384E+16   8.36623E+17   0.00000E+00   1.50746E+17   0.00000E+00   4.88358E+08
  3  RBLAN      5  RB      -2.95530E+18   4.61500E+17   3.29807E+18   0.00000E+00   8.04267E+17   0.00000E+00  -1.17054E+09
  4  CORE1      2  C1       4.07572E+17   7.49625E+17   4.35230E+18   0.00000E+00   5.50949E+18   0.00000E+00  -6.61003E+09
  5  CORE2      3  C2       4.48623E+18   2.11718E+18   1.08934E+19   0.00000E+00   1.74968E+19   0.00000E+00  -2.71839E+10
  6  ROD1A      7  EMPTY1  -7.06113E+16   2.21569E+14   7.03898E+16   0.00000E+00   0.00000E+00   0.00000E+00  -1.69794E+06
  7  ROD2A      8  EMPTY2  -1.26479E+17   3.96875E+14   1.26082E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.85408E+06
  8  ROD3A      9  EMPTY3  -1.17226E+17   3.67841E+14   1.16858E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.60942E+06
  9  ROD4A     10  EMPTY4  -6.83456E+16   2.14459E+14   6.81312E+16   0.00000E+00   0.00000E+00   0.00000E+00  -1.54602E+06
 10  ROD5A     11  EMPTY5  -9.63934E+16   3.02470E+14   9.60909E+16   0.00000E+00   0.00000E+00   0.00000E+00  -2.25480E+06
 11  ROD1B1    12  NOROD1  -6.85716E+15   2.15168E+13   6.83564E+15   0.00000E+00   0.00000E+00   0.00000E+00  -1.98394E+05
 12  ROD1B2    12  NOROD1  -4.80194E+15   1.50679E+13   4.78688E+15   0.00000E+00   0.00000E+00   0.00000E+00  -1.32190E+05
 13  ROD1B3    12  NOROD1  -1.83522E+15   5.75866E+12   1.82946E+15   0.00000E+00   0.00000E+00   0.00000E+00   5.80910E+04
 14  ROD1B4    12  NOROD1  -7.57339E+14   2.37643E+12   7.54962E+14   0.00000E+00   0.00000E+00   0.00000E+00   4.56735E+04
 15  ROD1B5    12  NOROD1  -2.98502E+14   9.36660E+11   2.97565E+14   0.00000E+00   0.00000E+00   0.00000E+00   1.74251E+04
 16  ROD1B6    12  NOROD1  -1.07440E+14   3.37132E+11   1.07103E+14   0.00000E+00   0.00000E+00   0.00000E+00   7.80136E+03
 17  ROD2B     13  NOROD2  -1.07973E+17   3.38806E+14   1.07635E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.36467E+06
 18  ROD3B     14  NOROD3  -1.17226E+17   3.67841E+14   1.16858E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.60933E+06
 19  ROD4B     15  NOROD4  -3.16059E+16   9.91752E+13   3.15067E+16   0.00000E+00   0.00000E+00   0.00000E+00  -6.81504E+05
 20  ROD5B     16  NOROD5  -3.55816E+15   1.11650E+13   3.54699E+15   0.00000E+00   0.00000E+00   0.00000E+00   2.73435E+04
     TOTALS                 7.39521E+16   3.42563E+18   2.04617E+19   0.00000E+00   2.39613E+19   0.00000E+00  -3.44984E+10
AREA  AREA                      NET    +  ABSORPTION +    SCATTER  -    SCATTER  -    FISSION  -    EXTERNAL =     BALANCE
NO.  NAME                     LEAKAGE       RATE(1)        OUT(2)          IN       PRODUCTION(3)    SOURCE
  1  ROD1B               -1.46576E+16   4.59936E+13   1.46116E+16   0.00000E+00   0.00000E+00   0.00000E+00  -2.01593E+05
…
```

Figure 2-13. The DIF3D Balance Edit Output Excerpt for the Base State

The balance edits in Figure 2-13 from DIF3D are intended to provide a region-wise breakdown of the operator into leakage, absorption, scattering, fission source, and external source. The last column indicates the error in the balance for each region noting that the balance edits are given for each energy group. In the balance edit output, it indicates how to merge the various terms to form the operator (leakage + absorption + scatter out – scatter in – fission production – external source). From the perturbation equation, the balance edit for the perturbed state needs to be obtained in addition to the balance edits for the base state when using the perturbed state flux solution and perturbed eigenvalue. This last aspect requires some knowledge of how to execute DIF3D as a restart calculation where the flux solution vectors are provided via binary interface files, the bypass execution mode is turned on, and the eigenvalue is initialized to the perturbed state values. This will cause DIF3D to produce the balance edits using the perturbed state flux solution. This is not shown here for brevity but is included in the supplementary documentation for this benchmark.

Because the balance edits are only produced on a region basis, the ROD1B region has to be broken into six regions for the six perturbed meshes (ROD1B1, ROD1B2, … ROD1B6). Figure 2-14 shows the balance edits for the first group of the base state but using the perturbed flux. What should be immediately clear is that the “Balance” column result is extremely large in many of the meshes compared with that observed in Figure 2-13. This is a strong indication that the flux solution being used is not consistent with the base state which is the desired behavior here.

```
…
DIF3D   11.3159 11/06/20            Some problem to run                                                    PAGE     23
REGION AND AREA BALANCE INTEGRALS FOR   REAL  K-EFF  PROBLEM WITH ENERGY RANGE (EV) =(8.006E+05,1.000E+07)  FOR GROUP    1
REGION     ZONE  ZONE         NET    +  ABSORPTION +    SCATTER  -    SCATTER  -    FISSION  -    EXTERNAL =    BALANCE
NO.  NAME    NO.  NAME       LEAKAGE       RATE(1)        OUT(2)          IN       PRODUCTION(3)    SOURCE
  1  REFL      6  RE      -3.34104E+17   5.50789E+15   3.28596E+17   0.00000E+00   0.00000E+00   0.00000E+00  -5.43322E+06
  2  ABLAN     4  AB      -7.59638E+17   8.76984E+16   8.20347E+17   0.00000E+00   1.48407E+17   0.00000E+00  -1.59333E+09
  3  RBLAN     5  RB      -2.97764E+18   4.65505E+17   3.32669E+18   0.00000E+00   8.14560E+17   0.00000E+00  -5.24831E+09
  4  CORE1     2  C1       3.98642E+17   7.46105E+17   4.33186E+18   0.00000E+00   5.47661E+18   0.00000E+00  -2.50919E+10
  5  CORE2     3  C2       4.53045E+18   2.13109E+18   1.09649E+19   0.00000E+00   1.76264E+19   0.00000E+00  -8.48804E+10
  6  ROD1A     7  EMPTY1  -7.12011E+16   2.23420E+14   7.09777E+16   0.00000E+00   0.00000E+00   0.00000E+00  -1.73574E+06
  7  ROD2A     8  EMPTY2  -1.28900E+17   4.04472E+14   1.28496E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.92341E+06
  8  ROD3A     9  EMPTY3  -1.19277E+17   3.74275E+14   1.18903E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.66446E+06
  9  ROD4A    10  EMPTY4  -6.89927E+16   2.16490E+14   6.87762E+16   0.00000E+00   0.00000E+00   0.00000E+00  -1.55696E+06
 10  ROD5A    11  EMPTY5  -9.72694E+16   3.05218E+14   9.69642E+16   0.00000E+00   0.00000E+00   0.00000E+00  -2.27320E+06
 11  ROD1B1   12  NOROD1  -2.08655E+16   1.66233E+13   5.28103E+15   0.00000E+00   0.00000E+00   0.00000E+00  -1.55678E+16
 12  ROD1B2   12  NOROD1  -1.29892E+16   1.03484E+13   3.28756E+15   0.00000E+00   0.00000E+00   0.00000E+00  -9.69133E+15
 13  ROD1B3   12  NOROD1  -4.76202E+15   3.79385E+12   1.20526E+15   0.00000E+00   0.00000E+00   0.00000E+00  -3.55296E+15
 14  ROD1B4   12  NOROD1  -1.65270E+15   1.31669E+12   4.18297E+14   0.00000E+00   0.00000E+00   0.00000E+00  -1.23309E+15
 15  ROD1B5   12  NOROD1  -5.32574E+14   4.24296E+11   1.34794E+14   0.00000E+00   0.00000E+00   0.00000E+00  -3.97356E+14
 16  ROD1B6   12  NOROD1  -1.43709E+14   1.14492E+11   3.63726E+13   0.00000E+00   0.00000E+00   0.00000E+00  -1.07222E+14
 17  ROD2B    13  NOROD2  -1.06420E+17   3.33933E+14   1.06086E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.31386E+06
 18  ROD3B    14  NOROD3  -1.16044E+17   3.64129E+14   1.15679E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.57285E+06
 19  ROD4B    15  NOROD4  -3.17330E+16   9.95740E+13   3.16334E+16   0.00000E+00   0.00000E+00   0.00000E+00  -6.87588E+05
 20  ROD5B    16  NOROD5  -3.45626E+15   1.08453E+13   3.44542E+15   0.00000E+00   0.00000E+00   0.00000E+00   2.86590E+04
     TOTALS               7.34689E+16   3.43827E+18   2.05237E+19   0.00000E+00   2.40660E+19   0.00000E+00  -3.05499E+16
AREA  AREA                    NET    +  ABSORPTION +    SCATTER  -    SCATTER  -    FISSION  -    EXTERNAL =    BALANCE
NO.  NAME                   LEAKAGE       RATE(1)        OUT(2)          IN       PRODUCTION(3)    SOURCE
  1  ROD1B              -4.09457E+16   3.26210E+13   1.03633E+16   0.00000E+00   0.00000E+00   0.00000E+00  -3.05498E+16
…
```

Figure 2-14. The DIF3D Balance Edit Output Excerpt for the Base State with the Perturbed Flux

The same detail can be obtained for the perturbed state an excerpt of which is shown in Figure 2-15. Note that the balance column is again 6 or more orders of magnitude lower than the other columns for every region in the domain. Focusing on the C1, C2, and ROD1B1 regions, one finds that the results between Figure 2-13 and Figure 2-15 for C1 and C2 are similar while that of ROD1B1 are all different.

```
…
DIF3D   11.3159 11/06/20            Some problem to run                                                    PAGE     40
REGION AND AREA BALANCE INTEGRALS FOR   REAL  K-EFF  PROBLEM WITH ENERGY RANGE (EV) =(8.006E+05,1.000E+07)  FOR GROUP    1
REGION     ZONE  ZONE         NET    +  ABSORPTION +    SCATTER  -    SCATTER  -    FISSION  -    EXTERNAL =    BALANCE
NO.  NAME    NO.  NAME       LEAKAGE       RATE(1)        OUT(2)          IN       PRODUCTION(3)    SOURCE
  1  REFL      6  RE      -3.33999E+17   5.50617E+15   3.28493E+17   0.00000E+00   0.00000E+00   0.00000E+00  -5.43123E+06
  2  ABLAN     4  AB      -7.59400E+17   8.76709E+16   8.20090E+17   0.00000E+00   1.48361E+17   0.00000E+00  -1.26479E+09
  3  RBLAN     5  RB      -2.97671E+18   4.65360E+17   3.32565E+18   0.00000E+00   8.14305E+17   0.00000E+00  -3.44615E+09
  4  CORE1     2  C1       3.98518E+17   7.45872E+17   4.33051E+18   0.00000E+00   5.47490E+18   0.00000E+00  -1.29784E+10
  5  CORE2     3  C2       4.52903E+18   2.13042E+18   1.09615E+19   0.00000E+00   1.76209E+19   0.00000E+00  -4.58919E+10
  6  ROD1A     7  EMPTY1  -7.11789E+16   2.23350E+14   7.09555E+16   0.00000E+00   0.00000E+00   0.00000E+00  -1.73520E+06
  7  ROD2A     8  EMPTY2  -1.28860E+17   4.04345E+14   1.28456E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.92246E+06
  8  ROD3A     9  EMPTY3  -1.19240E+17   3.74158E+14   1.18866E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.66368E+06
  9  ROD4A    10  EMPTY4  -6.89711E+16   2.16422E+14   6.87547E+16   0.00000E+00   0.00000E+00   0.00000E+00  -1.55648E+06
 10  ROD5A    11  EMPTY5  -9.72390E+16   3.05123E+14   9.69339E+16   0.00000E+00   0.00000E+00   0.00000E+00  -2.27246E+06
 11  ROD1B1   17  ROD     -2.08590E+16   1.49272E+15   1.93662E+16   0.00000E+00   0.00000E+00   0.00000E+00  -3.90840E+05
 12  ROD1B2   17  ROD     -1.29852E+16   9.29254E+14   1.20559E+16   0.00000E+00   0.00000E+00   0.00000E+00  -2.98096E+05
 13  ROD1B3   17  ROD     -4.76053E+15   3.40676E+14   4.41985E+15   0.00000E+00   0.00000E+00   0.00000E+00  -5.02820E+04
 14  ROD1B4   17  ROD     -1.65219E+15   1.18235E+14   1.53395E+15   0.00000E+00   0.00000E+00   0.00000E+00  -1.10782E+04
 15  ROD1B5   17  ROD     -5.32407E+14   3.81005E+13   4.94307E+14   0.00000E+00   0.00000E+00   0.00000E+00  -3.62012E+03
 16  ROD1B6   17  ROD     -1.43664E+14   1.02810E+13   1.33383E+14   0.00000E+00   0.00000E+00   0.00000E+00  -7.39125E+02
 17  ROD2B    13  NOROD2  -1.06387E+17   3.33828E+14   1.06053E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.31322E+06
 18  ROD3B    14  NOROD3  -1.16007E+17   3.64015E+14   1.15643E+17   0.00000E+00   0.00000E+00   0.00000E+00  -2.57205E+06
 19  ROD4B    15  NOROD4  -3.17231E+16   9.95428E+13   3.16236E+16   0.00000E+00   0.00000E+00   0.00000E+00  -6.87384E+05
 20  ROD5B    16  NOROD5  -3.45518E+15   1.08419E+13   3.44434E+15   0.00000E+00   0.00000E+00   0.00000E+00   2.86475E+04
     TOTALS               7.34459E+16   3.44009E+18   2.05450E+19   0.00000E+00   2.40585E+19   0.00000E+00  -6.36042E+10
AREA  AREA                    NET    +  ABSORPTION +    SCATTER  -    SCATTER  -    FISSION  -    EXTERNAL =    BALANCE
 NO.  NAME                   LEAKAGE       RATE(1)        OUT(2)          IN       PRODUCTION(3)    SOURCE
  1  ROD1B              -4.09329E+16   2.92927E+15   3.80037E+16   0.00000E+00   0.00000E+00   0.00000E+00  -7.54656E+05
…
```

Figure 2-15. The DIF3D Balance Edit Output Excerpt for the Perturbed State

The other components needed from the DIF3D output is the adjoint flux from the base state which is reported in the regular DIF3D output and not shown for brevity. To compute the perturbation, the group-wise balance edit detail needs to be summed together and collapsed with

the adjoint flux to produce a single value per mesh. It should be clear that by doing this, only the base state evaluated with the perturbed flux will actually contribute significantly to the reactivity worth as this amounts to multiplying the balance edit column by the adjoint flux for the perturbed state. This is also consistent with the perturbation equation and the transport operator.

Taking this approach for region ROD1B1 produces the results shown in Table 2-6 which are notably worse than the results in Table 2-5. The detailed calculation can be found in the companion supplementary information for this benchmark along with all of the DIF3D input and output files used to generate it. As can be seen, the mesh wise results are consistently higher using the balance edit approach than what PERSENT computes.

There are two issues with the balance edit approach that cause this to fail: 1) the denominator is crudely calculated and 2) the numerator is somewhat crudely calculated. The issue with the denominator is that PERSENT includes the spatial dependence of the forward and adjoint flux solutions within each mesh of a given region while the balance edit approach is done with a region wise sum of the components ignoring the mesh-wise combination of the forward and adjoint components. This of course completely misses the mesh-wise spatial dependence of the forward and adjoint flux along with the spatial dependence inside of each mesh. The magnitude of the denominator computed by PERSENT is 5.880E+29 while that with the balance edit is 5.4332E+29. Substituting in the denominator value from PERSENT will reduce the total worth from -510.64 to -495.58 pcm but neither is still close to the PERSENT value of -431.19. This indicates issues with the numerator. While it is technically being done mesh wise on this perturbation, it also does not consider the spatial dependence of the flux within those meshes and it is not hard to see that the numerator value in the balance edit approach does not agree with that of PERSENT. In that regard, the balance edit approach gets both the numerator and denominator incorrect and thus the worth is incorrect.

Overall, the balance edit approach will always fail unless the mesh can be refined such that the inherent flat flux approach is valid. Note that because DIF3D does not produce the balance edits on the mesh level, there is no way to get the denominator by hand although one can write a program to do it. Since the balance edit approach will never include the higher order aspects of the operator and their contribution to the perturbation worth, the direct approach should be considered more reliable.

Table 2-6. Control Rod Balance Edit Based Results for the DIF3D Consistency Check.

Axial Mesh	Balance Edit Worth (pcm)	PERSENT worth (pcm)
13	-290.1	-254.30
14	-142.3	-119.70
15	-54.24	-40.58
16	-17.76	-12.85
17	-5.326	-3.610
18	-0.8888	-0.1192
	-510.64	-431.19

It should be clear that the preceding approaches to doing hand calculations are not very accurate. The first approach using mesh-wise direct DIF3D perturbations is known to be limited but produced answers within 10% of the PERSENT reported worth. The hand calculation using the balance edits produces an answer that is 18% in error with the PERSENT reported worth and is known to only really work when the flux solution is roughly flat. Because each region in the balance table consists of many meshes, it is simply not a valid approach to computing the worth for this case. Since PERSENT computes the total worth correctly, and its mesh-wise result sums to that total worth correctly, it is reasonable to assume that the hand calculations here are incorrect. This is especially believable since the summation of the hand calculation applied does not sum to the correct total worth which is directly calculable with DIF3D.

2.2.3 *Manipulated NHFLUX Verification of the TEST3 Mesh-wise Worth*

From the preceding hand calculations, it should be obvious that getting an accurate hand calculation to verify the PERSENT mesh or region-wise results is difficult. Further, from the balance edit approach, it should be clear that using the average flux solution from the DIF3D output to compute the numerator for a single mesh will be inaccurate because it does not account for the spatial dependence of the forward and adjoint flux shape inside of that mesh.

One way around these issues is to manipulate the flux vector going into PERSENT such that it will force PERSENT to give a result consistent with the hand calculation. This can be done by using the forward_file, adjoint_file, and forward_pert_file input options of PERSENT. A utility program was created, included with the PERSENT distribution, which zeros out the higher order moments of the flux and current in the NHFLUX files. The same TEST3 problem from Figure 2-8 is used again in this verification work and both the diffusion and transport results are covered here for completeness.

The input and output changes are not important for this work other than to note that the mesh-wise flux and cross sections from the DIF3D output is used in the hand calculation of the numerator rather than the balance edit approach outlined above. The reason this approach is taken is because it will show the full calculation process where the balance edit approach hides the reaction rate calculation. Also, the denominator will again be calculated using the balance edit output, but the PERSENT one will be used because the balance edit approach is simply not accurate enough.

Table 2-7 provides the PERSENT calculated control rod reactivity worth and that worth resulting from the flat flux imposition. As can be seen, the flat flux modification significantly impacts the mesh-wise and total reactivity worth in both diffusion and transport calculations. Because the TEST3 perturbation focuses on replacing just a single composition, the operator evaluation is rather simple. To perform the hand calculation, the DIF3D flux results from the diffusion and transport calculations are needed along with the cross sections of the two compositions that make up the perturbation. Figure 2-16 provides the diffusion based forward and adjoint flux results for the base state along with the perturbed forward flux solution. Figure 2-17 provides the transport based forward and adjoint flux for the base state and the forward flux solution from the perturbed state. Figure 2-18 provides the cross sections for the two compositions involved in the TEST3 perturbation obtained from a ASCII dump of the COMPXS file.

The perturbation equation shown previously results the evaluation of the base operator $\langle \psi^*, B(\hat{\lambda})\hat{\psi} \rangle$ and perturbed operator $\langle \psi^*, \hat{B}(\hat{\lambda})\hat{\psi} \rangle$ with the perturbed eigenvalue. The diffusion theory k_{eff} result for the perturbed state was 0.89190880 while the transport one is 0.94947127.

Table 2-7. Impact of Flattening the Flux on the Mesh-wise Perturbation Worth.

	Diffusion (pcm)		Transport (pcm)	
Axial Mesh	Exact	Flat Flux	Exact	Flat Flux
13	-275	-329	-254	-284
14	-134	-168	-120	-139
15	-47.3	-71.9	-40.6	-53.1
16	-16.2	-25.2	-12.9	-17.4
17	-4.62	-7.74	-3.61	-5.21
18	-0.040	-1.39	-0.119	-0.870
Total	-477	-603	-431	-500

The cross sections from Figure 2-18 are arranged as seen in Table 2-8 to produce the cross section operator expression for the numerator. Since the higher order space-angle moments of the flux are zero, the entire flux-vector operation can be reduced to a matrix vector operation of this size for each mesh (3x3). Noting that both the forward and adjoint flux in Figure 2-16 contain the mesh volume, the operator application can be easily calculated as shown in the following equation for the first mesh ROD1B1 using the diffusion flux results from Figure 2-16. The volume of 7.8159E+2 cm^3 was taken from the DIF3D output noting that all of the meshes that were perturbed have the same volume for this problem.

$$\begin{pmatrix} 1.504E+13 \\ 1.305E+13 \\ 1.198E+13 \end{pmatrix}^T \cdot \begin{pmatrix} -2.905E-02 & 0 & 0 \\ 2.602E-02 & -2.865E-02 & 0 \\ 2.817E-04 & 1.742E-02 & -5.634E-02 \end{pmatrix} \cdot \begin{pmatrix} 6.585E+17 \\ 1.909E+18 \\ 1.311E+18 \end{pmatrix} \cdot \frac{1}{7.8159E+02}$$

$$= \begin{pmatrix} 1.504E+13 \\ 1.305E+13 \\ 1.198E+13 \end{pmatrix}^T \cdot \begin{pmatrix} -1.913E+16 \\ -3.756E+16 \\ -4.041E+16 \end{pmatrix} \cdot \frac{1}{7.8159E+02} = -1.615E+27 \qquad (3)$$

The remaining diffusion and transport based hand calculations can be carried out in the same manner and are provided in the EXCEL [12] document included with this benchmark. Table 2-9 provides the detailed calculation results of the hand calculation for the numerator in the diffusion problem which can be directly compared against the PERSENT output included as the last column in Table 2-9 and provided in Figure 2-19 for completeness. The denominator calculation is considerably more complicated than the numerator and using the balance edit approach the denominator for the diffusion theory problem is 4.58818E+29 while PERSENT reports it as 4.90703E+29. The difference here is purely the fact that the balance edit approach is not doing a sum consistent with the mesh-wise one in PERSENT. The mesh-wise worth computed using the hand calculated denominator is provided in Table 2-10 along with the mesh-wise worth calculated using the PERSENT denominator (labeled Alternate Worth). Clearly the worth computed using the PERSENT denominator and hand calculated numerator is very consistent with the PERSENT reported result (last column). When using the balance edit denominator, the error is of course directly the error in the dominator of 6%. While the hand calculated numerator value is identical

to the PERSENT one, the limited precision of the PERSENT output actually hides the small round off error that crops up in the hand calculation due to truncation error of the inputs.

Forward

REGION NO.	NAME	ZONE NO.	ZONE NAME	GROUP 1	GROUP 2	GROUP 3
1	REFL	6	RE	1.96136E+19	2.16133E+20	4.28917E+20
2	ABLAN	4	AB	3.97924E+19	1.89256E+20	2.37953E+20
3	RBLAN	5	RB	1.07566E+20	5.37145E+20	6.65618E+20
4	CORE1	2	C1	1.62600E+20	4.46351E+20	3.39098E+20
5	CORE2	3	C2	4.06219E+20	1.06758E+21	8.23898E+20
6	ROD1A	7	EMPTY1	7.96380E+18	2.40810E+19	2.01937E+19
7	ROD2A	8	EMPTY2	1.39136E+19	3.91542E+19	3.28756E+19
8	ROD3A	9	EMPTY3	1.29183E+19	3.65580E+19	3.09648E+19
9	ROD4A	10	EMPTY4	8.03828E+18	2.77668E+19	2.78283E+19
10	ROD5A	11	EMPTY5	1.13042E+19	3.85270E+19	3.79624E+19
11	ROD1B1	12	NOROD1	7.65550E+17	2.24764E+18	1.83100E+18
12	ROD1B2	12	NOROD1	5.28520E+17	1.67994E+18	1.51725E+18
13	ROD1B3	12	NOROD1	2.70940E+17	1.09791E+18	1.21344E+18
14	ROD1B4	12	NOROD1	1.12044E+17	6.35683E+17	8.96530E+17
15	ROD1B5	12	NOROD1	4.29561E+16	3.36108E+17	5.87650E+17
16	ROD1B6	12	NOROD1	1.58611E+16	1.50061E+17	2.82026E+17
17	ROD2B	13	NOROD2	1.19230E+19	3.39619E+19	2.90540E+19
18	ROD3B	14	NOROD3	1.29183E+19	3.65580E+19	3.09648E+19
19	ROD4B	15	NOROD4	3.73575E+18	1.30750E+19	1.33699E+19
20	ROD5B	16	NOROD5	4.69773E+17	2.31470E+18	3.23584E+18

Adjoint

1	REFL	6	RE	1.90036E+15	1.36390E+15	8.49477E+14
2	ABLAN	4	AB	1.42932E+15	1.12332E+15	8.54674E+14
3	RBLAN	5	RB	4.25175E+15	3.11893E+15	2.17270E+15
4	CORE1	2	C1	2.97533E+15	2.59870E+15	2.42117E+15
5	CORE2	3	C2	7.26579E+15	6.30572E+15	5.89350E+15
6	ROD1A	7	EMPTY1	1.61520E+14	1.39660E+14	1.27060E+14
7	ROD2A	8	EMPTY2	2.66038E+14	2.31119E+14	2.14397E+14
8	ROD3A	9	EMPTY3	2.48884E+14	2.15881E+14	1.99782E+14
9	ROD4A	10	EMPTY4	2.00099E+14	1.62880E+14	1.35207E+14
10	ROD5A	11	EMPTY5	2.76304E+14	2.25660E+14	1.88393E+14
11	ROD1B1	12	NOROD1	1.50422E+13	1.30502E+13	1.19788E+13
12	ROD1B2	12	NOROD1	1.15220E+13	9.79553E+12	8.69654E+12
13	ROD1B3	12	NOROD1	7.87362E+12	6.42379E+12	5.24367E+12
14	ROD1B4	12	NOROD1	4.86649E+12	3.81062E+12	2.85520E+12
15	ROD1B5	12	NOROD1	2.71899E+12	2.09599E+12	1.51894E+12
16	ROD1B6	12	NOROD1	1.33119E+12	9.66178E+11	6.53532E+11
17	ROD2B	13	NOROD2	2.31729E+14	2.00643E+14	1.85167E+14
18	ROD3B	14	NOROD3	2.48884E+14	2.15881E+14	1.99782E+14
19	ROD4B	15	NOROD4	9.46449E+13	7.68529E+13	6.35314E+13
20	ROD5B	16	NOROD5	1.84397E+13	1.40725E+13	1.03449E+13

Perturbed Forward

1	REFL	6	RE	1.95032E+19	2.14684E+20	4.23566E+20
2	ABLAN	4	AB	3.89750E+19	1.84474E+20	2.28040E+20
3	RBLAN	5	RB	1.08406E+20	5.40055E+20	6.67240E+20
4	CORE1	2	C1	1.62196E+20	4.44084E+20	3.33147E+20
5	CORE2	3	C2	4.08604E+20	1.07157E+21	8.23329E+20
6	ROD1A	7	EMPTY1	8.03638E+18	2.42710E+19	2.02100E+19
7	ROD2A	8	EMPTY2	1.41483E+19	3.97554E+19	3.33318E+19
8	ROD3A	9	EMPTY3	1.31186E+19	3.70762E+19	3.13573E+19
9	ROD4A	10	EMPTY4	8.10828E+18	2.79611E+19	2.79524E+19
10	ROD5A	11	EMPTY5	1.13972E+19	3.87652E+19	3.80798E+19
11	ROD1B1	17	ROD	6.58459E+17	1.90944E+18	1.31080E+18
12	ROD1B2	17	ROD	4.08362E+17	1.27336E+18	9.14211E+17
13	ROD1B3	17	ROD	1.84663E+17	7.60829E+17	6.57546E+17
14	ROD1B4	17	ROD	6.51374E+16	3.97963E+17	4.36974E+17
15	ROD1B5	17	ROD	2.18789E+16	1.97127E+17	2.63254E+17
16	ROD1B6	17	ROD	6.57454E+15	7.64715E+16	1.08741E+17
17	ROD2B	13	NOROD2	1.17681E+19	3.32954E+19	2.79473E+19
18	ROD3B	14	NOROD3	1.27978E+19	3.59746E+19	2.99218E+19
19	ROD4B	15	NOROD4	3.74677E+18	1.30431E+19	1.32127E+19
20	ROD5B	16	NOROD5	4.57811E+17	2.23894E+18	3.08522E+18

Figure 2-16. The DIF3D Diffusion Flux Excerpts for TEST3

Forward

REGION NO.	NAME	ZONE NO.	ZONE NAME	GROUP 1	GROUP 2	GROUP 3
1	REFL	6	RE	1.18145E+19	1.65595E+20	3.71428E+20
2	ABLAN	4	AB	2.77161E+19	1.60431E+20	2.16200E+20
3	RBLAN	5	RB	8.15968E+19	4.68943E+20	6.08947E+20
4	CORE1	2	C1	1.61938E+20	4.54962E+20	3.45900E+20
5	CORE2	3	C2	4.23809E+20	1.09137E+21	8.24977E+20
6	ROD1A	7	EMPTY1	7.14186E+18	2.37775E+19	2.05485E+19
7	ROD2A	8	EMPTY2	1.27925E+19	3.88842E+19	3.30467E+19
8	ROD3A	9	EMPTY3	1.18567E+19	3.62251E+19	3.10488E+19
9	ROD4A	10	EMPTY4	6.91270E+18	2.60153E+19	2.67181E+19
10	ROD5A	11	EMPTY5	9.74955E+18	3.62594E+19	3.66222E+19
11	ROD1B1	12	NOROD1	6.93556E+17	2.23266E+18	1.86907E+18
12	ROD1B2	12	NOROD1	4.85685E+17	1.63186E+18	1.50124E+18
13	ROD1B3	12	NOROD1	1.85620E+17	9.71780E+17	1.15720E+18
14	ROD1B4	12	NOROD1	7.65997E+16	5.25573E+17	8.10320E+17
15	ROD1B5	12	NOROD1	3.01915E+16	2.67306E+17	5.20561E+17
16	ROD1B6	12	NOROD1	1.08668E+16	1.12677E+17	2.36669E+17
17	ROD2B	13	NOROD2	1.09208E+19	3.35660E+19	2.90509E+19
18	ROD3B	14	NOROD3	1.18567E+19	3.62251E+19	3.10489E+19
19	ROD4B	15	NOROD4	3.19673E+18	1.21989E+19	1.27819E+19
20	ROD5B	16	NOROD5	3.59884E+17	1.95478E+18	2.87778E+18
	TOTALS			7.83145E+20	2.59214E+21	2.59729E+21

Adjoint

1	REFL	6	RE	1.75157E+15	1.36444E+15	8.92822E+14
2	ABLAN	4	AB	1.44416E+15	1.15396E+15	8.75099E+14
3	RBLAN	5	RB	4.37682E+15	3.27873E+15	2.28948E+15
4	CORE1	2	C1	3.48422E+15	2.95995E+15	2.68473E+15
5	CORE2	3	C2	8.49228E+15	7.20805E+15	6.57620E+15
6	ROD1A	7	EMPTY1	1.81524E+14	1.55837E+14	1.39446E+14
7	ROD2A	8	EMPTY2	2.98628E+14	2.57921E+14	2.35345E+14
8	ROD3A	9	EMPTY3	2.78826E+14	2.40606E+14	2.19097E+14
9	ROD4A	10	EMPTY4	2.13328E+14	1.76520E+14	1.45717E+14
10	ROD5A	11	EMPTY5	2.95679E+14	2.45145E+14	2.03345E+14
11	ROD1B1	12	NOROD1	1.69733E+13	1.45782E+13	1.31247E+13
12	ROD1B2	12	NOROD1	1.27789E+13	1.08345E+13	9.48507E+12
13	ROD1B3	12	NOROD1	8.12324E+12	6.73877E+12	5.46099E+12
14	ROD1B4	12	NOROD1	4.85086E+12	3.90876E+12	2.94557E+12
15	ROD1B5	12	NOROD1	2.62364E+12	2.13456E+12	1.58675E+12
16	ROD1B6	12	NOROD1	1.17702E+12	9.43343E+11	6.56628E+11
17	ROD2B	13	NOROD2	2.59024E+14	2.23291E+14	2.02849E+14
18	ROD3B	14	NOROD3	2.78826E+14	2.40606E+14	2.19097E+14
19	ROD4B	15	NOROD4	1.00487E+14	8.31112E+13	6.84066E+13
20	ROD5B	16	NOROD5	1.81364E+13	1.44860E+13	1.07788E+13
	TOTALS			2.15200E+16	1.76418E+16	1.47957E+16

Perturbed Forward

1	REFL	6	RE	1.17738E+19	1.64610E+20	3.66848E+20
2	ABLAN	4	AB	2.71683E+19	1.56269E+20	2.07040E+20
3	RBLAN	5	RB	8.22793E+19	4.71687E+20	6.10659E+20
4	CORE1	2	C1	1.61127E+20	4.51874E+20	3.39846E+20
5	CORE2	3	C2	4.26459E+20	1.09581E+21	8.24785E+20
6	ROD1A	7	EMPTY1	7.19927E+18	2.39388E+19	2.05593E+19
7	ROD2A	8	EMPTY2	1.30333E+19	3.95526E+19	3.35636E+19
8	ROD3A	9	EMPTY3	1.20603E+19	3.67954E+19	3.14912E+19
9	ROD4A	10	EMPTY4	6.97597E+18	2.62106E+19	2.68532E+19
10	ROD5A	11	EMPTY5	9.83508E+18	3.65027E+19	3.67557E+19
11	ROD1B1	17	ROD	5.35654E+17	1.73616E+18	1.22005E+18
12	ROD1B2	17	ROD	3.33457E+17	1.12536E+18	8.24032E+17
13	ROD1B3	17	ROD	1.22250E+17	6.15472E+17	5.64109E+17
14	ROD1B4	17	ROD	4.24279E+16	3.01160E+17	3.55680E+17
15	ROD1B5	17	ROD	1.36721E+16	1.41903E+17	2.08497E+17
16	ROD1B6	17	ROD	3.68927E+15	5.21897E+16	8.38492E+16
17	ROD2B	13	NOROD2	1.07603E+19	3.28696E+19	2.79394E+19
18	ROD3B	14	NOROD3	1.17334E+19	3.56268E+19	3.00119E+19
19	ROD4B	15	NOROD4	3.20858E+18	1.21769E+19	1.26362E+19
20	ROD5B	16	NOROD5	3.49469E+17	1.88479E+18	2.73363E+18
	TOTALS			7.85015E+20	2.58978E+21	2.57498E+21

Figure 2-17. The DIF3D Transport Flux Excerpts for TEST3

NOROD1

```
0                                        EDIT OF (NONFISSIONABLE  COMPOSITION NOROD1
          ICHI  =  0
0     GROUP    ABSORPTION        TOTAL          REMOVAL         TRANSPORT         NUP   NDN
        1     3.102396E-05   6.639006E-02   9.886960E-03   4.386690E-02         0     0
        2     1.354846E-05   8.467602E-02   3.055284E-03   7.510162E-02         0     1
        3     6.795118E-05   1.136947E-01   6.795118E-05   1.102576E-01         0     2
…
        1         1,  5.650324E-02
        2         1,  9.835166E-03   2,  8.162058E-02
        3         1,  2.076991E-05   2,  3.041736E-03   3,  1.136269E-01
```

ROD

```
0                                        EDIT OF (NONFISSIONABLE  COMPOSITION ROD
          ICHI  =  0
0     GROUP    ABSORPTION        TOTAL          REMOVAL         TRANSPORT         NUP   NDN
        1     2.786726E-03   2.256333E-01   3.894108E-02   1.846248E-01         0     0
        2     1.124429E-02   3.515438E-01   3.170062E-02   3.245980E-01         0     1
        3     5.640611E-02   4.590986E-01   5.640611E-02   4.406591E-01         0     2
…
        1         1,  1.866924E-01
        2         1,  3.585187E-02   2,  3.198436E-01
        3         1,  3.024830E-04   2,  2.045632E-02   3,  4.026923E-01
```

Figure 2-18. The DIF3D Cross Section Output Excerpt for the Numerator of TEST3

Table 2-8. The Numerator Base and Perturbed State Cross Section Operator Matrices.

Base State									
	Total			Scatter			Operator		
Group	1	2	3	1	2	3	1	2	3
1	6.639E-02	0.000E+00	0.000E+00	5.650E-02	0.000E+00	0.000E+00	9.887E-03	0.000E+00	0.000E+00
2	0.000E+00	8.468E-02	0.000E+00	9.835E-03	8.162E-02	0.000E+00	-9.835E-03	3.055E-03	0.000E+00
3	0.000E+00	0.000E+00	1.137E-01	2.077E-05	3.042E-03	1.136E-01	-2.077E-05	-3.042E-03	6.800E-05
Perturbed State									
1	2.256E-01	0.000E+00	0.000E+00	1.867E-01	0.000E+00	0.000E+00	3.894E-02	0.000E+00	0.000E+00
2	0.000E+00	3.515E-01	0.000E+00	3.585E-02	3.198E-01	0.000E+00	-3.585E-02	3.170E-02	0.000E+00
3	0.000E+00	0.000E+00	4.591E-01	3.025E-04	2.046E-02	4.027E-01	-3.025E-04	-2.046E-02	5.641E-02
Base - Perturbed									
						1	-2.905E-02	0.000E+00	0.000E+00
						2	2.602E-02	-2.864E-02	0.000E+00
						3	2.817E-04	1.741E-02	-5.634E-02

For the transport problem, the numerator calculated results are shown in Table 2-11 which can be directly compared against the PERSENT output (last column), also provided in Figure 2-19 for completeness. The denominator using the balance edit approach was computed as 5.40926E+29 while PERSENT reports it as 5.54039E+29 which is notably much closer than the diffusion theory result earlier. The balance edit approach is again inaccurate because of a inconsistent mesh-wise sum. The mesh-wise worth computed using the hand calculated denominator is provided in Table 2-12 along with the mesh-wise worth calculated using the PERSENT denominator (labeled Alternate Worth). The worth computed using the PERSENT denominator is again consistent with

the PERSENT reported result (last column). When using the balance edit denominator, the error is of course is directly the error in the dominator of 2%. The preceding work is sufficient to display that the mesh-wise perturbation results from PERSENT are understood, consistent with the manual, and accurate.

Table 2-9. Hand Calculation of the Mesh-Wise Numerator in Diffusion with a Flat Flux.

Region	Operator · Forward			Numerator	PERSENT Numerator
	Group 1	Group 2	Group 3		
ROD1B1	-1.913E+16	-3.756E+16	-4.041E+16	-1.615E+27	-1.615E+27
ROD1B2	-1.186E+16	-2.585E+16	-2.922E+16	-8.240E+26	-8.240E+26
ROD1B3	-5.365E+15	-1.699E+16	-2.374E+16	-3.530E+26	-3.530E+26
ROD1B4	-1.893E+15	-9.705E+15	-1.767E+16	-1.236E+26	-1.236E+26
ROD1B5	-6.357E+14	-5.077E+15	-1.139E+16	-3.797E+25	-3.797E+25
ROD1B6	-1.910E+14	-2.019E+15	-4.793E+15	-6.829E+24	-6.829E+24

Table 2-10. Hand Calculation of the Mesh-Wise Worth in Diffusion with a Flat Flux.

Region	Numerator	Worth	Worth (pcm)	Alternate Worth† (pcm)	PERSENT Worth (pcm)
ROD1B1	-1.615E+27	-3.519E-03	-352	-329	-329
ROD1B2	-8.240E+26	-1.796E-03	-180	-168	-168
ROD1B3	-3.530E+26	-7.693E-04	-76.9	-71.9	-71.9
ROD1B4	-1.236E+26	-2.695E-04	-26.95	-25.2	-25.2
ROD1B5	-3.797E+25	-8.275E-05	-8.28	-7.74	-7.74
ROD1B6	-6.829E+24	-1.488E-05	-1.49	-1.39	-1.39
		Total	-645	-599	-603

†Hand calculated worth uses denominator value from PERSENT

Table 2-11. Hand Calculation of the Mesh-Wise Numerator in Transport with a Flat Flux.

Region	Operator · Forward			Numerator	PERSENT Numerator
	Group 1	Group 2	Group 3		
ROD1B1	-1.556E+16	-3.580E+16	-3.835E+16	-1.573E+27	-1.573E+27
ROD1B2	-9.688E+15	-2.356E+16	-2.673E+16	-7.717E+26	-7.717E+26
ROD1B3	-3.552E+15	-1.445E+16	-2.103E+16	-2.940E+26	-2.940E+26
ROD1B4	-1.233E+15	-7.523E+15	-1.478E+16	-9.627E+25	-9.627E+25
ROD1B5	-3.972E+14	-3.709E+15	-9.271E+15	-2.887E+25	-2.887E+25
ROD1B6	-1.072E+14	-1.399E+15	-3.814E+15	-4.819E+24	-4.819E+24

The next part of the verification work to complete is verification of the balance edits components for PERSENT which are shown in Figure 2-19. The capture component is rather straightforward while the out-scatter and in-scatter terms are defined in the DIF3D manual to be:

$$\Sigma_{g,\text{out-scatter}} = \Sigma_{g,\text{removal}} - \Sigma_{g,\text{absorption}} + \Sigma_{g,n2n}$$
$$\Sigma_{g,g',in\text{-scatter}} = \Sigma_{s,g,g'} \cdot \left(1 - \delta_{g,g'}\right). \quad (4)$$

The out-scatter and in-scatter terms are not exactly what they imply by name with regard to the operator. These can be obtained from the regular DIF3D output as was done earlier in Figure 2-18 or can be obtained by using the PrintTables utility on the COMPXS file that DIF3D produces.

Table 2-12. Hand Calculation of the Mesh-Wise Worth in Transport with a Flat Flux.

Region	Numerator	Worth	Worth (pcm)	Alternate Worth† (pcm)	PERSENT Worth (pcm)
ROD1B1	-1.573E+27	-2.907E-03	-291	-284	-284
ROD1B2	-7.717E+26	-1.427E-03	-143	-139	-139
ROD1B3	-2.940E+26	-5.436E-04	-54.4	-53.1	-53.1
ROD1B4	-9.627E+25	-1.780E-04	-17.8	-17.4	-17.4
ROD1B5	-2.887E+25	-5.338E-05	-5.34	-5.21	-5.21
ROD1B6	-4.819E+24	-8.908E-06	-0.891	-0.870	-0.870
		Total	-512	-500	-500

†Hand calculated worth uses denominator value from PERSENT

For the capture component, the absorption cross section in Figure 2-18 is used because there is no fission in these materials. The operation itself is diagonal (like the total in Table 2-7) and thus rather easy to calculate. For diffusion theory result, one obtains

$$\frac{\begin{pmatrix}1.504E+13\\1.305E+13\\1.198E+13\end{pmatrix}^T \cdot \begin{pmatrix}-2.756E-02 & 0 & 0\\ 0 & -1.123E-02 & 0\\ 0 & 0 & -5.634E-02\end{pmatrix} \cdot \begin{pmatrix}6.585E+17\\1.909E+18\\1.311E+18\end{pmatrix}}{7.8159E+02} = -1.525E+27 \quad (5)$$

Taking this number and dividing by the PERSENT provided denominator value of 4.90703E+29 produces -3.107E-03 which matches the PERSENT diffusion theory reported result for ROD1B1 in Figure 2-19 of -3.107E-03. The remaining mesh-wise values can be calculated similarly and the results are summarized in Table 2-13 for both diffusion and transport. As can be seen, the capture results identically match those in Figure 2-19 for both diffusion and transport. Because the balance edit denominator will produce a consistent 6% error in diffusion theory and 2% error in transport, the results reported are only those using the PERSENT computed denominator.

From the scatter-out cross section definition, one should realize that it can be done similarly to the preceding capture calculation. Since both the removal and absorption cross sections are provided in Figure 2-18, no effort is taken to demonstrate how they are calculated here. For diffusion theory, the result for ROD1B1 is calculated as

$$\frac{\begin{pmatrix}1.504E+13\\1.305E+13\\1.198E+13\end{pmatrix}^T \cdot \begin{pmatrix}-2.630E-02 & 0 & 0\\ 0 & -1.741E-02 & 0\\ 0 & 0 & 0\end{pmatrix} \cdot \begin{pmatrix}6.585E+17\\1.909E+18\\1.311E+18\end{pmatrix}}{7.8159E+02} = -8.885E+26 \quad (6)$$

…

Diffusion

[PERSENT]...|Region|	Numerator	Numerator / Sum[Denominator]	= Leakage	+ Capture	+ Fission	+ Out Scatter	- In Scatter	- Production	|| n,2n
[PERSENT]...|REFL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ABLAN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|RBLAN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|CORE1	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|CORE2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD1A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD2A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD3A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD4A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD5A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD1B1|	-1.615E+27	-3.291E-03	2.421E-08	-3.107E-03	0.000E+00	-1.811E-03	-1.627E-03	0.000E+00	0.000E+00
[PERSENT]...|ROD1B2|	-8.240E+26	-1.679E-03	1.204E-08	-1.567E-03	0.000E+00	-8.890E-04	-7.768E-04	0.000E+00	0.000E+00
[PERSENT]...|ROD1B3|	-3.530E+26	-7.193E-04	4.409E-09	-6.600E-04	0.000E+00	-3.216E-04	-2.623E-04	0.000E+00	0.000E+00
[PERSENT]...|ROD1B4|	-1.236E+26	-2.520E-04	1.204E-09	-2.300E-04	0.000E+00	-9.059E-05	-6.857E-05	0.000E+00	0.000E+00
[PERSENT]...|ROD1B5|	-3.797E+25	-7.737E-05	2.731E-10	-7.126E-05	0.000E+00	-2.284E-05	-1.673E-05	0.000E+00	0.000E+00
[PERSENT]...|ROD1B6|	-6.829E+24	-1.392E-05	4.923E-11	-1.267E-05	0.000E+00	-3.955E-06	-2.703E-06	0.000E+00	0.000E+00
[PERSENT]...|ROD2B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD3B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD4B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD5B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

=PERSENT...Parameter General PT of TEST3 is -6.03244E-03 denominator 4.90703E+29 k-eff A 8.9572173E-01 F 8.9190882E-01

…

Transport

[PERSENT]...|Region|	Numerator	Numerator / Sum[Denominator]	= Leakage	+ Capture	+ Fission	+ Out Scatter	- In Scatter	- Production	|| n,2n
[PERSENT]...|REFL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ABLAN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|RBLAN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|CORE1	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|CORE2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD1A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD2A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD3A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD4A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD5A	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD1B1|	-1.573E+27	-2.839E-03	2.071E-08	-2.667E-03	0.000E+00	-1.497E-03	-1.325E-03	0.000E+00	0.000E+00
[PERSENT]...|ROD1B2|	-7.717E+26	-1.393E-03	9.898E-09	-1.297E-03	0.000E+00	-7.142E-04	-6.182E-04	0.000E+00	0.000E+00
[PERSENT]...|ROD1B3|	-2.940E+26	-5.307E-04	3.038E-09	-4.907E-04	0.000E+00	-2.165E-04	-1.765E-04	0.000E+00	0.000E+00
[PERSENT]...|ROD1B4|	-9.627E+25	-1.738E-04	7.280E-10	-1.603E-04	0.000E+00	-5.705E-05	-4.359E-05	0.000E+00	0.000E+00
[PERSENT]...|ROD1B5|	-2.887E+25	-5.211E-05	1.399E-10	-4.874E-05	0.000E+00	-1.369E-05	-1.032E-05	0.000E+00	0.000E+00
[PERSENT]...|ROD1B6|	-4.819E+24	-8.697E-06	2.174E-11	-8.073E-06	0.000E+00	-2.139E-06	-1.515E-06	0.000E+00	0.000E+00
[PERSENT]...|ROD2B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD3B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD4B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
[PERSENT]...|ROD5B	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

=PERSENT...Parameter General PT of TEST3 is -4.99677E-03 denominator 5.54039E+29 k-eff A 9.5337451E-01 F 9.4947129E-01

Figure 2-19. PERSENT Diffusion and Transport Perturbation Results for TEST3

Table 2-13. Hand Calculation of the Mesh-Wise Balance Edits.

	Diffusion							
Region	Capture	Worth	Scatter-out	Worth	Scatter-in	Worth	Total Worth	Leakage Error (%)
ROD1B1	-1.525E+27	-3.107E-03	-8.885E+26	-1.811E-03	-7.985E+26	-1.627E-03	-3.291E-03	-1.2%
ROD1B2	-7.689E+26	-1.567E-03	-4.362E+26	-8.890E-04	-3.812E+26	-7.768E-04	-1.679E-03	-0.9%
ROD1B3	-3.239E+26	-6.600E-04	-1.578E+26	-3.216E-04	-1.287E+26	-2.623E-04	-7.193E-04	-0.4%
ROD1B4	-1.128E+26	-2.300E-04	-4.445E+25	-9.059E-05	-3.365E+25	-6.857E-05	-2.520E-04	0.3%
ROD1B5	-3.497E+25	-7.126E-05	-1.121E+25	-2.284E-05	-8.210E+24	-1.673E-05	-7.737E-05	0.8%
ROD1B6	-6.215E+24	-1.267E-05	-1.941E+24	-3.955E-06	-1.327E+24	-2.703E-06	-1.392E-05	1.2%
	Transport							
ROD1B1	-1.478E+27	-2.667E-03	-8.293E+26	-1.497E-03	-7.343E+26	-1.325E-03	-2.839E-03	-0.8%
ROD1B2	-7.185E+26	-1.297E-03	-3.957E+26	-7.142E-04	-3.425E+26	-6.182E-04	-1.393E-03	-0.7%
ROD1B3	-2.719E+26	-4.907E-04	-1.200E+26	-2.165E-04	-9.777E+25	-1.765E-04	-5.307E-04	0.2%
ROD1B4	-8.882E+25	-1.603E-04	-3.161E+25	-5.705E-05	-2.415E+25	-4.359E-05	-1.738E-04	0.6%
ROD1B5	-2.701E+25	-4.874E-05	-7.585E+24	-1.369E-05	-5.717E+24	-1.032E-05	-5.211E-05	0.8%
ROD1B6	-4.473E+24	-8.073E-06	-1.185E+24	-2.139E-06	-8.392E+23	-1.515E-06	-8.697E-06	1.3%

Dividing this number by the PERSENT denominator yields -1.811E-03 which exactly matches the result from PERSENT in Figure 2-19. The other mesh-wise scatter-out components can be calculated similarly and the results are summarized in Table 2-13. From the cross section definition, the scatter-in component only considers the non-diagonal part of the scattering matrix. For the ROD1B1 region the hand calculation for the diffusion theory results is

$$\frac{\begin{pmatrix}1.504E+13\\1.305E+13\\1.198E+13\end{pmatrix}^{T}\cdot\begin{pmatrix}0 & 0 & 0\\-2.602E-02 & 0 & 0\\-2.817E-02 & -1.742E-02 & 0\end{pmatrix}\cdot\begin{pmatrix}6.585E+17\\1.909E+18\\1.311E+18\end{pmatrix}}{7.8159E+02} = -7.985E+26. \quad (7)$$

Dividing this result by the PERSENT denominator yields -1.627E-03 which matches the result from PERSENT in Figure 2-19. The remaining regions are calculated in the excel document provided with this benchmark and are summarized in Table 2-13.

The last non-zero term in the balance table is the leakage. Noting that in DIF3D, the balance edit includes a balance column as seen in Figure 2-15. In PERSENT, no balance column is provided and the manual clearly indicates that the leakage component is calculated as the balance of the remaining terms as defined by the equation in the PERSENT output of Figure 2-19. It is a trivial matter to verify that the provided values sum to numbers similar to those reported by PERSENT but they have larger errors which are reported in Table 2-13 as the leakage term results (error instead of absolute value). From Figure 2-19, one can see that the leakage magnitude for each mesh is 4-5 orders below the other column results. Since the higher order spatial moments were eliminated when the NHFLUX file was modified, this causes the leakage component to be approximately zero in all cases. In the PERSENT output for the non-modified NHFLUX case, the leakage component is of course not zero. Since the leakage in that case is still calculated as the balance of the other components, there is no additional verification work required for the leakage term as the small ~1% errors observed on the hand calculation demonstrate the consistency of the solution within the limits of the truncation error on the inputs to the hand calculation.

For completeness, the approach used to compute the denominator is displayed. Since the denominator only considers the fission related part of the operator, only the principle cross sections are needed, which are provided for the fissionable regions in Figure 2-20. The balance edit output is obtained by the special restart case of the base state model of DIF3D using the perturbed flux solution and is given in Figure 2-21. The transport output table was truncated for brevity as the only regions that matter are those which are fissionable (C1, C2, AB, RB). To compute the denominator value using this output, the fission production column of output in Figure 2-21 is combined with the adjoint flux from Figure 2-16, the region volume (1.40686E+05 which can be found in the DIF3D base state output), the χ cross section from Figure 2-20, and the perturbed state eigenvalue of 0.8919088. For the diffusion theory result, the C1 contribution to the denominator is calculated as

$$\frac{\begin{pmatrix}2.97533E+15\\2.59870E+15\\2.42117E+15\end{pmatrix}^{T}\cdot\begin{pmatrix}7.80677E-01\\2.10399E-01\\8.9008E-03\end{pmatrix}\cdot 7.38310E+18\cdot 0.8919088}{1.40686E+05} = 1.35323E+29. \quad (8)$$

As can be seen, a full matrix operation is not needed as was the case with the previous hand claculations. It is easy to show that the fission source product is easy to calculation given the cross section data and the forward flux from the perturbed state. This is because the balance edit table output is produced by simply taking the cross section data for the zone assigned to the region and multiplying by the region total flux. The volume of this mesh is notably much larger than the

ROD1D1 region appearing in the previous examples. Applying this approach for region C2, AB, and RB yields the denominator values reported earlier. Since the region-wise denominator contribution is not broken down in the PERSENT output, no additional effort is spent on this test problem for verification.

C1

0 EDIT OF (FISSIONABLE) COMPOSITION C1

…

0 GROUP	ABSORPTION	TOTAL	REMOVAL	TRANSPORT	FISSION	NU*FISSION	CHI	NUP NDN	
1	4.629085E-03	1.759774E-01	3.150540E-02	1.282202E-01	3.946822E-03	1.173647E-02	7.806772E-01	0	0
2	2.953306E-03	2.271875E-01	1.011564E-02	2.025138E-01	1.714146E-03	5.003071E-03	2.103988E-01	0	1
3	8.187719E-03	3.032856E-01	8.187719E-03	2.946599E-01	2.560147E-03	7.376363E-03	8.908197E-03	0	2

C2

0 EDIT OF (FISSIONABLE) COMPOSITION C2

…

0 GROUP	ABSORPTION	TOTAL	REMOVAL	TRANSPORT	FISSION	NU*FISSION	CHI	NUP NDN	
1	4.995597E-03	1.708081E-01	3.069904E-02	1.241903E-01	4.381792E-03	1.324595E-02	7.811701E-01	0	0
2	3.508110E-03	2.191331E-01	1.038254E-02	1.954908E-01	2.336343E-03	6.819576E-03	2.099283E-01	0	1
3	9.047873E-03	2.941941E-01	9.047873E-03	2.858489E-01	3.490728E-03	1.005776E-02	8.885806E-03	0	2

AB

0 EDIT OF (FISSIONABLE) COMPOSITION AB

…

0 GROUP	ABSORPTION	TOTAL	REMOVAL	TRANSPORT	FISSION	NU*FISSION	CHI	NUP NDN	
1	3.226951E-03	1.964958E-01	3.341245E-02	1.434344E-01	2.404944E-03	6.632042E-03	7.753020E-01	0	0
2	1.317413E-03	2.500613E-01	9.136459E-03	2.231909E-01	2.715176E-06	6.717427E-06	2.155300E-01	0	1
3	5.233314E-03	3.364296E-01	5.233314E-03	3.266579E-01	9.160641E-07	2.212597E-06	9.152390E-03	0	2

RB

0 EDIT OF (FISSIONABLE) COMPOSITION RB

…

0 GROUP	ABSORPTION	TOTAL	REMOVAL	TRANSPORT	FISSION	NU*FISSION	CHI	NUP NDN

Figure 2-20. The DIF3D Cross Section Excerpt for the Denominator of TEST3

Diffusion

REGION NO.	NAME	ZONE NO.	ZONE NAME	NET LEAKAGE	+ ABSORPTION RATE(1)	+ SCATTER OUT(2)	- SCATTER IN	- FISSION PRODUCTION(3)	EXTERNAL SOURCE	= BALANCE
1	REFL	6	RE	-6.09468E+17	6.09468E+17	1.78189E+18	1.78189E+18	0.00000E+00	0.00000E+00	-1.23312E+07
2	ABLAN	4	AB	-1.26821E+18	1.56276E+18	2.61982E+18	2.62251E+18	2.91864E+17	0.00000E+00	1.58654E+09
3	RBLAN	5	RB	-6.31874E+18	7.80419E+18	1.02563E+19	1.02698E+19	1.47190E+18	0.00000E+00	5.61909E+09
4	CORE1	2	C1	2.60064E+18	4.79176E+18	7.54261E+18	7.55190E+18	7.38310E+18	0.00000E+00	5.15412E+10
5	CORE2	3	C2	1.03197E+19	1.32545E+19	1.78753E+19	1.78956E+19	2.35540E+19	0.00000E+00	1.20516E+11
6	ROD1A	7	EMPTY1	-1.95215E+15	1.95214E+15	1.53087E+17	1.53087E+17	0.00000E+00	0.00000E+00	-1.20104E+06
7	ROD2A	8	EMPTY2	-3.24366E+15	3.24365E+15	2.60463E+17	2.60463E+17	0.00000E+00	0.00000E+00	-1.08147E+06
8	ROD3A	9	EMPTY3	-3.04117E+15	3.04116E+15	2.42158E+17	2.42158E+17	0.00000E+00	0.00000E+00	-7.58884E+05
9	ROD4A	10	EMPTY4	-2.53069E+15	2.53068E+15	1.65024E+17	1.65024E+17	0.00000E+00	0.00000E+00	-7.19781E+05
10	ROD5A	11	EMPTY5	-3.46761E+15	3.46760E+15	2.30326E+17	2.30326E+17	0.00000E+00	0.00000E+00	-1.60075E+06
11	ROD1B1	12	NOROD1	-9.72772E+16	1.35417E+14	1.23021E+16	1.23021E+16	0.00000E+00	0.00000E+00	-9.71417E+16
12	ROD1B2	12	NOROD1	-6.70471E+16	9.20757E+13	7.90084E+15	7.90084E+15	0.00000E+00	0.00000E+00	-6.69550E+16
13	ROD1B3	12	NOROD1	-4.61757E+16	6.07397E+13	4.13574E+15	4.13574E+15	0.00000E+00	0.00000E+00	-4.61149E+16
14	ROD1B4	12	NOROD1	-2.93148E+16	3.71188E+13	1.85315E+15	1.85315E+15	0.00000E+00	0.00000E+00	-2.92777E+16
15	ROD1B5	12	NOROD1	-1.71328E+16	2.12456E+13	8.15537E+14	8.15537E+14	0.00000E+00	0.00000E+00	-1.71115E+16
16	ROD1B6	12	NOROD1	-7.01437E+15	8.63222E+12	2.97511E+14	2.97511E+14	0.00000E+00	0.00000E+00	-7.00573E+15
17	ROD2B	13	NOROD2	-2.71622E+15	2.71621E+15	2.17339E+17	2.17339E+17	0.00000E+00	0.00000E+00	-2.07034E+05
18	ROD3B	14	NOROD3	-2.91871E+15	2.91870E+15	2.35643E+17	2.35643E+17	0.00000E+00	0.00000E+00	-5.29608E+05
19	ROD4B	15	NOROD4	-1.19120E+15	1.19120E+15	7.66288E+16	7.66288E+16	0.00000E+00	0.00000E+00	-7.81855E+04
20	ROD5B	16	NOROD5	-2.54273E+14	2.54272E+14	1.13265E+16	1.13265E+16	0.00000E+00	0.00000E+00	8.02794E+05
	TOTALS			4.43862E+18	2.80444E+19	4.16952E+19	4.17410E+19	3.27009E+19	0.00000E+00	-2.63606E+17

Transport

…

2	ABLAN	4	AB	-1.18419E+18	1.37748E+18	2.04260E+18	2.04447E+18	1.91415E+17	0.00000E+00	-2.04443E+09
3	RBLAN	5	RB	-5.93645E+18	6.99735E+18	8.45599E+18	8.46628E+18	1.05062E+18	0.00000E+00	-6.81940E+09
4	CORE1	2	C1	2.15985E+18	4.86448E+18	7.56935E+18	7.57858E+18	7.01509E+18	0.00000E+00	-3.21125E+10
5	CORE2	3	C2	9.14348E+18	1.34414E+19	1.85003E+19	1.85214E+19	2.25638E+19	0.00000E+00	-1.08603E+11

Figure 2-21. The DIF3D Balance Table Output for the Denominator Calculation in TEST3

2.2.4 *Manipulated NHFLUX File Verification of a Simple Test*

As demonstrated in the verification of the mesh-wise worth of TEST3 above, a large perturbation is difficult to hand calculate. The use of DIF3D to approximately calculate the worth

by calculating individual mesh-wise perturbations was also shown to be inaccurate and difficult to use as every mesh must be named uniquely. In this section, a new problem is introduced which is considerably simpler than that shown in Figure 2-1 as seen in Figure 2-22. In this simple problem, There are only three fuel meshes and thus the numerator and denominator are rather easy to hand calculate. The DIF3D test cases discussed here are benchmark 46 in the DIF3D distribution while the PERSENT test cases are benchmark 24 in the PERSENT distribution.

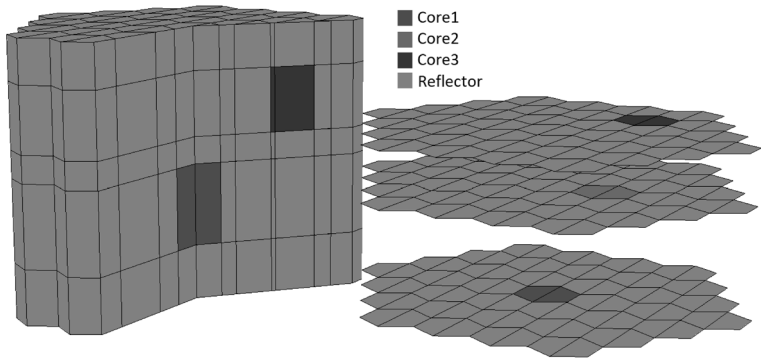

Figure 2-22. The DIF3D Geometry Layout of the Simple Test Problem

The DIF3D input for this problem is provided in Figure 2-23. As can be seen, the three fueled regions are named CORE1, CORE2, and CORE3 and are surrounded by a single reflector region (REFL). The entire problem consists of 4 radial rings of hexes and only has 5 axial meshes. Each axial mesh has a different size to better demonstrate the importance of volume on the worth calculation. The fuel compositions are very similar to those in Figure 2-3 but the actinide densities are increased significantly.

```
03  120
04  4  4  4  4  4  4
09 Z  1  10.0
09 Z  1  25.0
09 Z  1  30.0
09 Z  1  42.0
09 Z  1  50.0
14  C1   PU239  0.020    U238  0.01
14  C1   NA     0.0104   FE    0.0181    O-16  0.0149
14   C2  PU239  0.020    U238  0.01
14   C2  NA     0.0104   FE    0.0181    O-16  0.0149
14  C3   PU239  0.020    U238  0.01
14  C3   NA     0.0104   FE    0.0181    O-16  0.0149
14   C1A PU239  0.021    U238  0.015
14   C1A NA     0.0103   FE    0.0180    O-16  0.0148
14  RE   NA     0.0044   FE    0.0691
15    RE     REFL
15    C1     CORE1
15    C2     CORE2
15    C3     CORE3
29  9.5
30  REFL    1   0  0  0.0 50.0
30  REFL    2   0  0  0.0 50.0
30  REFL    3   0  0  0.0 50.0
30  REFL    4   0  0  0.0 50.0
30  CORE1   1   0  0 10.0 25.0
30  CORE2   2   1  1 25.0 30.0
30  CORE3   3   3  3 30.0 42.0
```

Figure 2-23. The A.NIP3 Input for the Simple Test Verification Work

The PERSENT perturbation input is shown in Figure 2-24 and it defines the perturbation to only replace the composition in CORE1 and CORE3. This means the numerator will only consider these two meshes for the calculation while the denominator will consider all three meshes. Only a transport calculation is used on this test problem as the preceding work demonstrates that both diffusion and transport are handled properly by PERSENT. The DIF3D exact perturbation results are provided in Table 2-14 along with the PERSENT calculated perturbation worth and that resulting from imposing a flat flux input.

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   ./dif3d.x
DIF3D_INPUT        ./dif3d_a.inp
ADJUST_ZONE      TEST1 GENERALIZED_PT C1 C1A
ADJUST_ZONE      TEST1 GENERALIZED_PT C3 C1A
PROBLEM_EDITS    TEST1 PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
```

Figure 2-24. The PERSENT Input for the Simple Test Verification Work

Table 2-14. DIF3D and PERSENT Perturbation Results for the Simple Test.

	DIF3D		PERSENT	
			Exact (pcm)	Flat (pcm)
Base	0.99807 6	Worth (pcm)		
C1 → C1A	1.05060 1	5009		
C3 → C1A	1.00346 3	537.9		
C1 & C3 → C1A	1.05248 1	5179.2	5179.3	2768

Also included in Table 2-14 are the results of performing the two mesh perturbations separately. As can be seen, the DIF3D approach to computing the mesh wise worth by separate perturbations leads to 5547 pcm (5009 + 537.9) which is 368 pcm higher than the exact result or 7% in error. The PERSENT calculated result is nearly identical to the exact result but the flat flux result is 2411 pcm below the correct result or 46% in error. As discussed previously, this aspect is not important as the goal is to reproduce the PERSENT calculated values using a hand calculation.

The DIF3D adjoint flux for the base state and forward flux for the perturbed state are provided in Figure 2-25 along with the volumes of each region as calculated by DIF3D. To complete the hand calculation, the macroscopic cross section data is needed which is provided in Figure 2-26 which were obtained with the PrintTables utility program. Note that only two sets of cross sections are provided as three of the compositions were identical (C1, C2, and C3). The base operator for the numerator assuming a flat flux system can be calculated from the preceding described data as

$$\begin{pmatrix} 0.340412 & 0 & 0 \\ 0 & 0.44526 & 0 \\ 0 & 0 & 0.628779 \end{pmatrix} - \begin{pmatrix} 0.252422 & 0 & 0 \\ 0.046022 & 0.399003 & 0 \\ 1.09646\text{E-}3 & 0.0100105 & 0.54946 \end{pmatrix} - \frac{\begin{pmatrix} 0.782033 \\ 0.209105 \\ 8.84662\text{E-}3 \end{pmatrix} \begin{pmatrix} 0.125214 \\ 0.0908756 \\ 0.134086 \end{pmatrix}^T}{1.05248101}$$

$$= \begin{pmatrix} -5.0487\text{E-}03 & -6.7524\text{E-}02 & -9.9631\text{E-}02 \\ -7.0899\text{E-}02 & 2.8202\text{E-}02 & -2.6640\text{E-}02 \\ -2.1489\text{E-}03 & -1.0774\text{E-}02 & 7.8192\text{E-}02 \end{pmatrix}. \quad (9)$$

Note that the perturbed eigenvalue is used with the fission source definition.

Base Adjoint

REGION NO.	NAME	ZONE NO.	ZONE NAME	GROUP 1	GROUP 2	GROUP 3
1	REFL	5	RE	1.86417E+14	1.74557E+14	1.89133E+14
2	CORE1	1	C1	2.05602E+13	1.81496E+13	2.10844E+13
3	CORE2	2	C2	3.11499E+12	2.76175E+12	3.19053E+12
4	CORE3	3	C3	4.84970E+12	4.29326E+12	4.93427E+12
	TOTALS			2.14942E+14	1.99761E+14	2.18343E+14

Perturbed Forward

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	REFL	5	RE	1.42093E+05	1.90472E+21	1.57873E+17	1.20888E+21	1.39055E+17
2	CORE1	1	C1	1.17238E+03	1.98546E+20	2.15595E+17	1.73337E+20	1.90684E+17
3	CORE2	2	C2	3.90794E+02	2.69667E+19	8.28338E+16	2.21139E+19	6.63782E+16
4	CORE3	3	C3	9.37906E+02	4.39812E+19	5.60288E+16	3.76267E+19	4.85975E+16
	TOTALS			1.44594E+05	2.17421E+21	2.15595E+17	1.44196E+21	1.90684E+17

…

REGION NO.	NAME	ZONE NO.	ZONE NAME	GROUP 1	GROUP 2	GROUP 3
1	REFL	5	RE	3.29583E+20	9.72222E+20	6.02913E+20
2	CORE1	1	C1	9.10374E+19	9.09974E+19	1.65110E+19
3	CORE2	2	C2	1.07637E+19	1.25497E+19	3.65333E+18
4	CORE3	3	C3	1.92752E+19	2.02909E+19	4.41511E+18
	TOTALS			4.50659E+20	1.09606E+21	6.27493E+20

Figure 2-25. The DIF3D Adjoint and Forward Flux Output Edit for the Simple Test

…

Base State Cross Sections (C1, C2, & C3)

```
[COMPXS]...CROSS SECTION DATA FOR COMPOSITION ORDERED.....................................................  1
[COMPXS]...   GROUP   TRANS (P1)   TOTAL (P0)    ABSORP.      REMOVAL        N2N        FISSION    YIELD/FISS  ....
[COMPXS]...       1  2.38216E-01  3.40412E-01  4.09986E-02  8.79922E-02  1.24893E-04  3.97856E-02  1.25214E-01 ....
[COMPXS]...       2  3.81551E-01  4.45260E-01  3.62501E-02  4.62606E-02  0.00000E+00  3.11302E-02  9.08756E-02 ....
[COMPXS]...       3  6.13120E-01  6.28779E-01  7.93156E-02  7.93156E-02  0.00000E+00  4.65359E-02  1.34086E-01 ....
[COMPXS]...ICHI =      1 FOR COMPOSITION.....................................................  1
[COMPXS]...             CHI   1     CHI
[COMPXS]...       1 7.82033E-01
[COMPXS]...       2 2.09105E-01
[COMPXS]...       3 8.84662E-03
…
[COMPXS]...SCATTERING MATRIX FOR LEGENDRE ORDER.....................................................  0
[COMPXS]...      TO GROUP   1  TO GROUP   2  TO GROUP   3  TO GROUP
[COMPXS]...   1  2.52422E-01   4.60220E-02   1.09646E-03
[COMPXS]...   2  0.00000E+00   3.99003E-01   1.00105E-02
[COMPXS]...   3  0.00000E+00   0.00000E+00   5.49460E-01
```

…

Perturbed State Cross Sections (C1A)

```
 [COMPXS]...CROSS SECTION DATA FOR COMPOSITION ORDERED.....................................................  4
[COMPXS]...   GROUP   TRANS (P1)   TOTAL (P0)    ABSORP.      REMOVAL        N2N        FISSION    YIELD/FISS  ....
[COMPXS]...       1  2.66693E-01  3.83531E-01  4.46971E-02  9.89631E-02  1.69914E-04  4.31276E-02  1.35206E-01 ....
[COMPXS]...       2  4.29307E-01  5.03973E-01  3.86825E-02  4.97377E-02  0.00000E+00  3.26882E-02  9.54232E-02 ....
[COMPXS]...       3  6.93837E-01  7.11744E-01  8.59688E-02  8.59688E-02  0.00000E+00  4.88633E-02  1.40792E-01 ....
[COMPXS]...ICHI =      1 FOR COMPOSITION.....................................................  4
[COMPXS]...             CHI   1     CHI
[COMPXS]...       1 7.81965E-01
[COMPXS]...       2 2.09170E-01
[COMPXS]...       3 8.84970E-03
[COMPXS]...SCATTERING MATRIX FOR LEGENDRE ORDER.....................................................  0
[COMPXS]...      TO GROUP   1  TO GROUP   2  TO GROUP   3  TO GROUP
[COMPXS]...   1  2.84571E-01   5.31549E-02   1.28106E-03
[COMPXS]...   2  0.00000E+00   4.54238E-01   1.10552E-02
[COMPXS]...   3  0.00000E+00   0.00000E+00   6.25770E-01
```

Figure 2-26. The Base and Perturbed Macroscopic Cross Sections for the Simple Test

The perturbed state can be calculated similarly, and the operator difference for the numerator is

$$\begin{pmatrix} \text{-3.5543E-03} & \text{3.3729E-03} & \text{4.9737E-03} \\ \text{9.1264E-03} & \text{-2.5686E-03} & \text{1.3410E-03} \\ \text{2.6898E-04} & \text{1.0832E-03} & \text{-6.5982E-03} \end{pmatrix}. \quad (10)$$

Applying the forward and adjoint flux for region CORE1 to this operator (along with dividing by the volume) produces

$$\frac{\begin{pmatrix}2.0560E+13\\1.8150E+13\\2.1084E+13\end{pmatrix}^T\begin{pmatrix}-3.5543E-03 & 3.3729E-03 & 4.9737E-03\\9.1264E-03 & -2.5686E-03 & 1.3410E-03\\2.6898E-04 & 1.0832E-03 & -6.5982E-03\end{pmatrix}\begin{pmatrix}9.1037E+19\\9.0997E+19\\1.6511E+19\end{pmatrix}}{1172.38} = 1.0989E+28. \quad (11)$$

Applying the forward and adjoint flux for region CORE3 to this operator (along with dividing by the volume) produces

$$\frac{\begin{pmatrix}4.8497E+12\\4.2933E+12\\4.9343E+12\end{pmatrix}^T\begin{pmatrix}-3.5543E-03 & 3.3729E-03 & 4.9737E-03\\9.1264E-03 & -2.5686E-03 & 1.3410E-03\\2.6898E-04 & 1.0832E-03 & -6.5982E-03\end{pmatrix}\begin{pmatrix}1.9275E+19\\2.0291E+19\\4.4151E+18\end{pmatrix}}{937.906} = 6.9660E+26. \quad (12)$$

The PERSENT calculated result for the flat flux input is given in Figure 2-27. As can be seen, the preceding two numerator values are very similar to the PERSENT reported values of 1.099E+28 for CORE1 and 6.965E+26 for CORE3. Summing the two results and dividing by the PERSENT calculated denominator of 4.22085E+29 produces a worth of 2.76845E-02 which is similar to the PERSENT result of 2.76822E-02 (0.01% error).

```
[PERSENT]...Region edits for General PT of TEST1
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |           | Sum[Denominator] |          |           |           |              |              |              |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|
[PERSENT]...|CORE1 |  1.099E+28|         2.603E-02| 1.706E-04|-7.310E-03|-1.948E-02|   -3.117E-02|  -2.858E-02|   -5.523E-02|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|
[PERSENT]...|CORE3 |  6.965E+26|         1.650E-03| 1.063E-05|-5.146E-04|-1.260E-03|   -1.958E-03|  -1.800E-03|   -3.572E-03|
=PERSENT...Parameter General PT of TEST1    is  2.76822E-02 denominator  4.22085E+29 k-eff A 9.9807453E-01 F  1.0524811E+00
…
[PERSENT]...|Region||   n,2n   |
[PERSENT]...|      ||         |
[PERSENT]...|REFL  || 0.000E+00|
[PERSENT]...|CORE1 ||-1.703E-04|
[PERSENT]...|CORE2 || 0.000E+00|
[PERSENT]...|CORE3 ||-1.063E-05|
```

Figure 2-27. The PERSENT Results for the Simple Test with Flat Flux Inputs

For the denominator, the base state fission source operator needs to be calculated which can be obtained with

$$\begin{pmatrix}0.782033\\0.209105\\8.84662E-3\end{pmatrix}\begin{pmatrix}0.125214\\0.0908756\\0.134086\end{pmatrix}^T. \quad (13)$$

This can be applied to the adjoint and forward fluxes of the three regions of interest to produce

$$CORE1 \quad \frac{1}{1172.38}\begin{pmatrix}2.0560E+13\\1.8150E+13\\2.1084E+13\end{pmatrix}^T\begin{pmatrix}0.782033\\0.209105\\8.84662E-3\end{pmatrix}\begin{pmatrix}0.125214\\0.0908756\\0.134086\end{pmatrix}^T\begin{pmatrix}9.1037E+19\\9.0997E+19\\1.6511E+19\end{pmatrix} = 3.7443E+29$$

$$CORE2 \quad \frac{1}{390.794}\begin{pmatrix}3.1150E+12\\2.7618E+12\\3.1905E+12\end{pmatrix}^T\begin{pmatrix}0.782033\\0.209105\\8.84662E-3\end{pmatrix}\begin{pmatrix}0.125214\\0.0908756\\0.134086\end{pmatrix}^T\begin{pmatrix}1.0764E+19\\1.2550E+19\\3.6533E+18\end{pmatrix} = 2.3180E+28$$

$$CORE3 \quad \frac{1}{937.906}\begin{pmatrix}4.8497E+12\\4.2933E+12\\4.9343E+12\end{pmatrix}^T\begin{pmatrix}0.782033\\0.209105\\8.84662E-3\end{pmatrix}\begin{pmatrix}0.125214\\0.0908756\\0.134086\end{pmatrix}^T\begin{pmatrix}1.9275E+19\\2.0291E+19\\4.4151E+18\end{pmatrix} = 2.4477E+28$$

3.7443E+29+2.3180E+28+2.4477E+28=4.2209E+29. (14)

The region values cannot be verified as PERSENT does not report that aspect, thus only the total value can be compared. From Figure 2-27, the hand calculated value of 4.22086E+29 compares well to the 4.22085E+29 value reported by PERSENT.

In summary, all of the hand calculations in this section demonstrate that PERSENT is calculating the perturbation worth consistent with the perturbation equation it states it is using. While the higher order spatial and angular basis functions were not fully verified as they require a complex matrix-vector system, the preceding work is sufficient to demonstrate that artificially setting the higher order moments to zero results in PERSENT producing the expected result. Beyond this aspect, the fact that the PERSENT calculated worth matches the exact perturbation worth for a wide variety of problems beyond those shown here, is indicative of the fact that the matrix-vector setup internal to PERSENT is consistent with that implemented in DIF3D and that required by the perturbation equation. It is important to note that none of the preceding work verified whether anisotropic scattering was handled properly by PERSENT. Given that many examples are provided with the PERSENT software distribution that demonstrate it is working correctly (PERSENT worth again matches the exact perturbation worth), it is reasonable to assume that anisotropic scattering is properly handled by PERSENT and does not need to be checked specifically. This is further justified as PERSENT does not produce specific output for the anisotropic scattering aspect. The same logic applies for the other cross section data inputs (inelastic scattering, (n,proton), (n,deuteron), etc…) many of which were not directly testable with the PERSENT output (lumped into capture). With this stated, the preceding work completes verification of task b) of Category 2 in Table 1-1.

2.2.5 *Verification of the Isotopic Mass Change and worth/kg*

The SAS4A software [13] requires a very specific form of the reactivity coefficients, worth/kg. An output feature of PERSENT is the ability to calculate the worth/kg on both a mesh and region-wise basis to simplify the input setup of SAS4A and thus it is verified here.

There are two basic aspects to consider for the calculation in PERSENT: 1) determination of unique isotopes and 2) calculation of the isotopic mass and mass change. The first aspect has to deal with the specific output produced by PERSENT for the isotopic breakdown. The second aspect deals with the mass change tables produced by PERSENT and thus is the modification of the worth tables produced by PERSENT using the mass calculated. For this section, the benchmark specified by Figure 2-1 and Figure 2-3 will be used. The PERSENT test case is benchmark 25 in the PERSENT distribution and benchmark 47 is a separate test of the base DIF3D model.

Figure 2-28 shows the perturbation input specified for this problem. To trigger the mass edit, the “PRINT_BY_MASS” keyword needs to be added to the PROBLEM_EDITS input of PERSENT as seen. In the first perturbation, the control rod positions are all filled with control rod material. In the second perturbation, both C1 and C2 materials are replaced with the C1P material. Because these perturbations involve different sets of isotopes, the two perturbations should be sufficient to fully verify the worth/kg feature.

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   ./dif3d.x
DIF3D_INPUT        ./dif3d_a.inp

ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD1 ROD
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD2 ROD
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD3 ROD
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD4 ROD
ADJUST_ZONE      TEST1 GENERALIZED_PT NOROD5 ROD
PROBLEM_EDITS    TEST1 PRINT_BY_REGION PRINT_BY_MESH PRINT_BY_MASS PRINT_BALANCE

ADJUST_ZONE      TEST2 GENERALIZED_PT C1 C1P
ADJUST_ZONE      TEST2 GENERALIZED_PT C2 C1P
PROBLEM_EDITS    TEST2 PRINT_BY_REGION PRINT_BY_MESH PRINT_BY_MASS PRINT_BALANCE
```

Figure 2-28. The PERSENT Input for the Worth/kg Verification

The PERSENT output for isotopic mass for the two perturbation theory problems is provided in Figure 2-29. Looking at Figure 2-3, the NOROD1 to NOROD5 materials only contain NA (NA23 5 in the PERSENT output) while the ROD material adds Fe, O-16, B-10, and C. The output for the TEST1 perturbation indicates a drop in the sodium density and increase in the other isotopes.

```
…
[PERSENT].....................................................................
[PERSENT]...Problem TEST1           is a zone perturbation using GENERALIZED_PT
[PERSENT]...Associated DIF3D output is P_dif3d_problem0001.out
[PERSENT].....................................................................
[PERSENT]...Replacing zone     NOROD1   with copy of zone     ROD
[PERSENT]...Replacing zone     NOROD2   with copy of zone     ROD
[PERSENT]...Replacing zone     NOROD3   with copy of zone     ROD
[PERSENT]...Replacing zone     NOROD4   with copy of zone     ROD
[PERSENT]...Replacing zone     NOROD5   with copy of zone     ROD
[PERSENT]...This perturbation has total core changes in mass of
[PERSENT]...NA23 5           -30.1116 kg
[PERSENT]...FE   5           114.1318 kg
[PERSENT]...O-16 5            26.9109 kg
[PERSENT]...B-10 5            10.1753 kg
[PERSENT]...C    5            55.8245 kg
…
[PERSENT].....................................................................
[PERSENT]...Problem TEST2           is a zone perturbation using GENERALIZED_PT
[PERSENT]...Associated DIF3D output is P_dif3d_problem0002.out
[PERSENT].....................................................................
[PERSENT]...Replacing zone     C1       with copy of zone     C1P
[PERSENT]...Replacing zone     C2       with copy of zone     C1P
[PERSENT]...This perturbation has total core changes in mass of
[PERSENT]...NA23 5           -10.7413 kg
[PERSENT]...O-16 5            13.7014 kg
[PERSENT]...PU239S           -74.4616 kg
[PERSENT]...U-238S           185.3736 kg
…
```

Figure 2-29. The PERSENT Isotopic Mass Change Output Excerpt for the Worth/kg Test

Given the sodium density is 0.022 in NOROD1 to NOROD5 and 0.0104 in ROD, these results are qualitatively consistent with the expected behavior. To calculate the mass change, one must have the isotopic mass and Avogadro's number. The isotopic mass information is included in the ISOTXS data file used by DIF3D and the excerpt of input is provided in Figure 2-30 while the Avogadro number used in PERSENT is $0.602214179 \cdot 10^{24}$.

```
…
4D  NA23 5 ENDF/B NA23 5
 2.29895E+01 0.0         1.11249E-12 1.20000E+03 0.0         0.0
…
4D  FE   5 ENDF/B FE   5
 5.58447E+01 0.0         1.24675E-12 1.20000E+03 0.0         0.0
…
4D  O-16 5 ENDF/B O-16 5
 1.59954E+01 0.0         5.40259E-13 1.20000E+03 0.0         0.0
…
4D  B-10 5 ENDF/B B-10 5
 1.00129E+01 0.0         4.45954E-13 1.20000E+03 0.0         0.0
…
4D  C    5 ENDF/B C    5
 1.20000E+01 0.0         7.91208E-13 1.20000E+03 0.0         0.0
…
4D  PU239S ENDF/B PU239S
 2.39053E+02 3.17282E-11 1.04375E-12 1.20000E+03 0.0         0.0
…
4D  U-238S ENDF/B U-238S
 2.38051E+02 3.09930E-11 9.09490E-13 1.20000E+03 0.0         0.0
…
```

Figure 2-30. An Excerpt from the ISOTXS Input Displaying the Isotopic Masses

The other aspect to know is the total volume involved in the perturbation which is provided in Figure 2-31. For the TEST1 perturbation, NOROD1 to NOROD5 are all perturbed and thus the total volume is 6.7998E+04 cm^3. For the TEST2 perturbation, both C1 and C2 are perturbed and thus the total volume is 6.0964E+05 cm^3. The total mass change for the TEST1 perturbation is provided in Table 2-15 while TEST2 is provided in Table 2-16

```
…
     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  REFL      6  RE          1.92271E+06      5.48837E+20      1.38239E+15      1.61582E+20      5.02274E+14
      2  ABLAN     4  AB          2.43855E+05      4.04347E+20      3.90248E+15      1.72813E+20      2.05527E+15
      3  RBLAN     5  RB          8.53494E+05      1.15949E+21      4.52104E+15      5.05719E+20      2.56540E+15
      4  CORE1     2  C1          1.40686E+05      9.62801E+20      8.92876E+15      5.73416E+20      5.31719E+15
      5  CORE2     3  C2          4.68953E+05      2.34015E+21      8.31708E+15      1.41086E+21      5.10659E+15
      6  ROD1A     7  EMPTY1      9.37906E+03      5.14679E+19      8.88255E+15      2.86468E+19      5.19479E+15
      7  ROD2A     8  EMPTY2      2.18845E+04      8.47235E+19      7.56199E+15      4.79603E+19      4.55448E+15
      8  ROD3A     9  EMPTY3      2.11029E+04      7.91306E+19      7.56199E+15      4.46194E+19      4.55448E+15
      9  ROD4A    10  EMPTY4      2.73556E+04      5.96461E+19      4.64105E+15      3.04415E+19      2.64786E+15
     10  ROD5A    11  EMPTY5      3.51715E+04      8.26312E+19      4.64105E+15      4.25433E+19      2.64786E+15
     11  ROD1B    12  NOROD1      4.68953E+03      1.33194E+19      6.81058E+15      6.67557E+18      3.95456E+15
     12  ROD2B    13  NOROD2      2.03213E+04      7.35377E+19      7.56199E+15      4.12786E+19      4.55448E+15
     13  ROD3B    14  NOROD3      2.11029E+04      7.91307E+19      7.56199E+15      4.46194E+19      4.55448E+15
     14  ROD4B    15  NOROD4      1.48502E+04      2.81775E+19      4.64105E+15      1.42297E+19      2.64786E+15
     15  ROD5B    16  NOROD5      7.03429E+03      5.19244E+18      2.81048E+15      2.12783E+18      1.54476E+15
…
```

Figure 2-31. DIF3D Output Excerpt Displaying the Region Volumes

For TEST1, the NOROD1 to NOROD5 materials used in the base state all have identical Na atom densities and thus the mass calculation is rather easy. As can be seen, the calculated isotopic mass change matches that reported by PERSENT in Figure 2-29 within the round off error on the calculation. The total mass change is 176.931 kg for this perturbation. For TEST2, the C1 and CP1 compositions are not actually different and thus the perturbation only really impacts C2. Also observable in Table 2-16 is that the Fe isotope mass change is zero as the atom density does not change between the C2 and CP1 compositions. As was the case for TEST1, the TEST2 mass change matches the result reported by PERSENT in Figure 2-29 within round of error. The total mass change is 113.8723 kg for TEST2.

Table 2-15. TEST1 Perturbation Isotopic Mass Change.

		Base State (NOROD 1-5)		Perturbed State (ROD)		Mass change (kg)
Isotope	Atom Mass	Atom Density	Mass (kg)	Atom Density	Mass (kg)	
NA23 5	22.990	0.0220	57.108	0.0104	26.997	-30.1116
FE 5	55.845			0.0181	114.132	114.1319
O-16 5	15.995			0.0149	26.911	26.9109
B-10 5	10.013			0.0090	10.175	10.1753
C 5	12.000			0.0412	55.825	55.8245
						176.931

The mesh-wise, region-wise, and area summary edits for mass change are calculated on a mesh-wise basis in PERSENT and reported as part of the regular output. Because of the expansive amount of mesh-wise data in the output, plane 14 is arbitrarily selected for explicit verification here, the excerpt of which is given in Figure 2-32 for TEST1 and TEST2. Note that the mesh-wise output was truncated to only those columns with non-zero parts. Since each mesh has the identical composition change, the only difference between the mesh-wise and total domain change is the actual volume of the mesh versus the total domain volume. Because every axial mesh has the same height (10 cm) in this test case and this is a hexagonal test case, the volume of each mesh is easily calculated to be 781.588 cm^3. Given the total volume of the perturbation was 6.7998E+04 cm^3, the mass change for each affected mesh should be

$$\frac{781.588}{67998} \cdot 176.9310 = 2.03369kg. \quad (15)$$

Table 2-16. TEST1 Perturbation Isotopic Mass Change.

		Base (C1)		Base (C2)		Perturbed (CP1)		Mass Change (kg)
Isotope	Atom Mass	Atom Density	Mass (kg)	Atom Density	Mass (kg)	Atom Density	Mass (kg)	
PU239S	239.05	0.0011	61.4309	0.0015	279.2311	0.0011	266.2004	-74.4616
U-238S	238.05	0.0064	355.9179	0.0054	1001.0185	0.0064	1542.3103	185.3738
NA23 5	22.99	0.0104	55.8551	0.0110	196.9249	0.0104	242.0386	-10.7414
FE 5	55.84	0.0181	236.1350	0.0181	787.1163	0.0181	1023.2513	0.0000
O-16 5	16.00	0.0149	55.6777	0.0138	171.8908	0.0149	241.2699	13.7014
								113.8723

Inspection of the mesh-wise results in Figure 2-32 match this result within round off error. For the region-wise result, the same volume ratio applies. Given the volumes are provided in Figure 2-31, it is a simple matter to compute the mass change for each region. As an example, for region ROD1B, the calculation is

$$\frac{4689.53}{67998} \cdot 176.9310 = 12.202kg. \quad (16)$$

This result is also within round off error of the result reported by PERSENT in Figure 2-32. The remaining ROD2B to ROD5B results match those in Figure 2-32 and are not displayed for

brevity. Also of note is that the total parameter value of 176.931 kg in Figure 2-32 matches the hand calculation in Table 2-15.

The TEST2 mesh and region-wise edits for mass are also given in Figure 2-32. As was the case with TEST1, the mesh-wise results are truncated. Noting that all of the mesh-wise results are identical, only one needs to be verified which is done for C2 as

$$\frac{781.588}{609639} \cdot 113.8723 = 0.18979kg. \quad (17)$$

This result matches the PERSENT reported value in Figure 2-32. It is important to note that the volume of C2 is used, rather than the CORE1+CORE2 volume as the non-zero mesh values shown in Figure 2-32 only correspond to the CORE2 region. All of the CORE1 mesh values are also displayed in Figure 2-32 but are all zero as expected. The region and total parameter value are identical in this perturbation as CORE2 (C2) is the only modified region and both are seen to match the hand calculated value of 113.8723 kg in Table 2-16.

```
…
[PERSENT]...Axial plane     14 data for mass(kg) change for TEST1
                7          8          9         10         11         12         13         14         15
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.034E+00
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  2.034E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits for mass(kg) change for TEST1
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|ABLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|RBLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD1A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD2A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD1B |  0.000E+00|         1.220E+01|
[PERSENT]...|ROD2B |  0.000E+00|         5.288E+01|
[PERSENT]...|ROD3B |  0.000E+00|         5.491E+01|
[PERSENT]...|ROD4B |  0.000E+00|         3.864E+01|
[PERSENT]...|ROD5B |  0.000E+00|         1.830E+01|
=PERSENT...Parameter mass(kg) change for TEST1 is  1.76931E+02
…
[PERSENT]...Axial plane     14 data for mass(kg) change for TEST2
                5          6          7          8          9         10         11         12         13         14         15
  15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  1.898E-01  0.000E+00
  14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01
  13  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01
  12  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01
  11  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01
  10  0.000E+00  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  0.000E+00
   9  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00
   8  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00
   7  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00
   6  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00
   5  0.000E+00  1.898E-01  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
 [PERSENT]...Region edits for mass(kg) change for TEST2
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|ABLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|RBLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |  0.000E+00|         1.139E+02|
[PERSENT]...|ROD1A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD2A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5A |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD1B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD2B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4B |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5B |  0.000E+00|         0.000E+00|
=PERSENT...Parameter mass(kg) change for TEST2        is  1.13872E+02
```

Figure 2-32. The Mesh and Region-wise Mass Change Excerpt for TEST1 and TEST2

The next aspect to check is the worth/kg value which is reported by PERSENT in mesh-wise, region-wise, and area-wise tables along with a total value. Conceptually, the desired result is to take each worth and divide by the relative mass change associated with the worth. Thus for the mesh-wise worth/kg, the mesh-wise worth is divided by the mesh-wise mass change. For the region-wise worth/kg, the region-wise worth is divided by the region-wise mass change. The area and total worth/kg are calculated in a consistent manner. Figure 2-33 provides the truncated mesh-wise (again for the 14th axial plane), region-wise, and total value perturbation results reported by PERSENT. The first section is the mass change, the second is the worth, and the third is the worth/kg as indicated by the various headers.

```
…
[PERSENT]...Axial plane     14 data for mass(kg) change for TEST1
                7          8          9         10         11         12         13         14         15
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.034E+00
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  2.034E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  2.034E+00  0.000E+00  0.000E+00  2.034E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits for mass(kg) change for TEST1
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|ROD1B |  0.000E+00|         1.220E+01|
[PERSENT]...|ROD2B |  0.000E+00|         5.288E+01|
[PERSENT]...|ROD3B |  0.000E+00|         5.491E+01|
[PERSENT]...|ROD4B |  0.000E+00|         3.864E+01|
[PERSENT]...|ROD5B |  0.000E+00|         1.830E+01|
=PERSENT...Parameter mass(kg) change for TEST1        is  1.76931E+02
…
[PERSENT]...Axial plane     14 data for General PT of TEST1
                7          8          9         10         11         12         13         14         15
    15   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.267E-04
    14   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13   0.000E+00  0.000E+00  0.000E+00 -6.347E-04  0.000E+00  0.000E+00 -5.642E-04  0.000E+00  0.000E+00
    12   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  -6.513E-04  0.000E+00  0.000E+00 -9.041E-04  0.000E+00  0.000E+00 -5.063E-04  0.000E+00 -9.667E-05
     9   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  -5.710E-04  0.000E+00  0.000E+00 -5.220E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits for General PT of TEST1
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |           | Sum[Denominator] |           |          |          |              |             |              |
[PERSENT]...|ROD1B | -1.889E+27|        -3.376E-03| 6.660E-04|-3.767E-03| 0.000E+00|   -2.145E-03|  -1.869E-03|    0.000E+00|
[PERSENT]...|ROD2B | -1.603E+28|        -2.865E-02| 2.595E-03|-2.954E-02| 0.000E+00|   -1.831E-02|  -1.661E-02|    0.000E+00|
[PERSENT]...|ROD3B | -1.791E+28|        -3.201E-02| 2.705E-03|-3.284E-02| 0.000E+00|   -2.035E-02|  -1.847E-02|    0.000E+00|
[PERSENT]...|ROD4B | -2.361E+27|        -4.220E-03| 2.230E-03|-5.907E-03| 0.000E+00|   -3.464E-03|  -2.921E-03|    0.000E+00|
[PERSENT]...|ROD5B | -1.102E+26|        -1.970E-04| 1.820E-04|-3.440E-04| 0.000E+00|   -1.720E-04|  -1.369E-04|    0.000E+00|
=PERSENT...Parameter General PT of TEST1  is -6.84519E-02 denominator  5.59401E+29 k-eff A  9.5337451E-01 F  8.9496809E-01
…
                7          8          9         10         11         12         13         14         15
    15   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -6.230E-05
    14   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13   0.000E+00  0.000E+00  0.000E+00 -3.121E-04  0.000E+00  0.000E+00 -2.774E-04  0.000E+00  0.000E+00
    12   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  -3.202E-04  0.000E+00  0.000E+00 -4.446E-04  0.000E+00  0.000E+00 -2.489E-04  0.000E+00 -4.753E-05
     9   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  -2.808E-04  0.000E+00  0.000E+00 -2.567E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits/mass(kg) for General PT of TEST1
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |           | Sum[Denominator] |           |          |          |              |             |              |
[PERSENT]...|ROD1B | -1.548E+26|        -2.767E-04| 5.458E-05|-3.087E-04| 0.000E+00|   -1.758E-04|  -1.532E-04|    0.000E+00|
[PERSENT]...|ROD2B | -3.031E+26|        -5.418E-04| 4.907E-05|-5.587E-04| 0.000E+00|   -3.463E-04|  -3.141E-04|    0.000E+00|
[PERSENT]...|ROD3B | -3.261E+26|        -5.830E-04| 4.927E-05|-5.981E-04| 0.000E+00|   -3.705E-04|  -3.363E-04|    0.000E+00|
[PERSENT]...|ROD4B | -6.109E+25|        -1.092E-04| 5.771E-05|-1.529E-04| 0.000E+00|   -8.964E-05|  -7.559E-05|    0.000E+00|
[PERSENT]...|ROD5B | -6.022E+24|        -1.076E-05| 9.944E-06|-1.879E-05| 0.000E+00|   -9.395E-06|  -7.480E-06|    0.000E+00|
=PERSENT...Parameter General PT of TEST1    is -3.86885E-04 denominator  5.59401E+29 k-eff A  9.5337451E-01 F  8.9496809E-01
```

Figure 2-33. The PERSENT Worth/kg Excerpt for TEST1

To calculate the worth/kg, one simply takes the worth value of interest and divides by the corresponding mass change value for that worth value. For the mesh-wise worth of -6.513E-04 at row 10, column 7, the mass change is 2.034 kg and thus the mesh-wise worth/kg is calculated as

$$\frac{\text{-6.5130E-04}}{\text{2.034 kg}} = \text{-3.2021E-04 kg}^{-1}. \quad (18)$$

This result closely matches the -3.202E-04 result reported by PERSENT in Figure 2-33 within round-off error. The remaining mesh-wise values were checked and all results were accurate within the round-off error of the provided numbers. These results are not included here for brevity but can be found in the excel document provided with the verification test problem (bench25).

The region-wise values in Figure 2-33 are calculated in a similar fashion. For region ROD3B, the worth of -3.201E-02 and the mass change of 54.91 kg are combined to give the worth/kg of

$$\frac{\text{-3.201E-02}}{\text{54.91 kg}} = \text{-5.8295E-04 kg}^{-1}. \quad (19)$$

This result is consistent with the PERSENT reported result of -5.830E-04 within round off error of the provided numbers. The last check is the total worth/kg result which takes the total worth of -6.84519E-02 and mass change of 176.931 kg to get

$$\frac{\text{-6.84519E-02}}{\text{176.931 kg}} = \text{-3.86885E-04 kg}^{-1}. \quad (20)$$

This result exactly matches the result reported by PERSENT as is expected. As can be seen, given the worth and mass change are calculated correctly by PERSENT, the worth/kg is a simple manipulation of the two computed results.

The TEST2 results for worth/kg are checked next and the PERSENT output excerpt is provided in Figure 2-34. Looking at the row 9 column 6 mesh-wise worth of -1.049E-04 and corresponding mass change of 0.1898 kg, the worth/kg can be calculated as

$$\frac{\text{-1.049E-04}}{\text{0.1898 kg}} = \text{-5.5269E-04 kg}^{-1}. \quad (21)$$

This result closely matches the -5.525E-04 result from PERSENT within round off error. The region and total worth are the same in this case because only region C2 was modified. Taking the total worth of -1.42515E-01 and mass change of 113.872 kg, the total worth/kg is

$$\frac{\text{-1.42515E-01}}{\text{113.872 kg}} = \text{-1.2515E-03 kg}^{-1}. \quad (22)$$

This result matches the CORE2 region result of -1.252E-03 and total worth/kg of -1.2515E-03 result. The remaining mesh-wise results on this plane were verified to be accurate but are not included here for brevity.

From all of the previous hand calculations of the mass, it should be clear that the calculation of mass change is a rather trivial operation. Looking at the source code of PERSENT, it uses a single subroutine to calculate the mass which relies upon the GEODST, NDXSRF, and ZNATDN files to be properly prepared by DIF3D and the unique isotope list to be properly identified by PERSENT. Given the former aspect was rigorously tested in the DIF3D verification work, it is reasonable to assume that the existing algorithm works for all test cases and no further verification work is needed beyond that shown above. For the isotope list, the PERSENT manual clearly indicates that the isotopes are collected by unique HABSID labels provided by the user in the ISOTXS dataset. This same sorting process is used in the UQ routines of PERSENT and will be verified later as part of the sensitivity verification work as that is where the isotope mapping information is provided to the user. Given that the worth/kg is a simple modification of the worth results from PERSENT, tasks c) and d) of category 2 can be considered verified with the preceding work.

```
…
[PERSENT]...Axial plane     14 data for mass(kg) change for TEST2
              5          6          7          8          9         10         11         12         13         14         15
  15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  1.898E-01  0.000E+00
  14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01
  13  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01
  12  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01
  11  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01
  10  0.000E+00  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  0.000E+00
   9  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00
   8  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00
   7  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01  0.000E+00  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00
   6  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00
   5  0.000E+00  1.898E-01  1.898E-01  1.898E-01  1.898E-01  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits for mass(kg) change for TEST2
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE2 |  0.000E+00|         1.139E+02|
=PERSENT...Parameter mass(kg) change for TEST2        is  1.13872E+02
…
[PERSENT]...Axial plane     14 data for General PT of TEST2
              5          6          7          8          9         10         11         12         13         14         15
  15   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -5.432E-05 -6.594E-05 -6.594E-05 -5.432E-05  0.000E+00
  14   0.000E+00  0.000E+00  0.000E+00  0.000E+00 -5.432E-05 -8.125E-05 -1.049E-04 -1.133E-04 -1.049E-04 -8.125E-05 -5.432E-05
  13   0.000E+00  0.000E+00  0.000E+00 -6.594E-05 -1.049E-04  0.000E+00 -1.517E-04 -1.517E-04  0.000E+00 -1.049E-04 -6.594E-05
  12   0.000E+00  0.000E+00 -6.594E-05 -1.133E-04 -1.517E-04  0.000E+00  0.000E+00  0.000E+00 -1.517E-04 -1.133E-04 -6.594E-05
  11   0.000E+00 -5.432E-05 -1.049E-04 -1.517E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.517E-04 -1.049E-04 -5.432E-05
  10   0.000E+00 -8.125E-05  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -8.125E-05  0.000E+00
   9  -5.432E-05 -1.049E-04 -1.517E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.517E-04 -1.049E-04 -5.432E-05  0.000E+00
   8  -6.594E-05 -1.133E-04 -1.517E-04  0.000E+00  0.000E+00  0.000E+00 -1.517E-04 -1.133E-04 -6.594E-05  0.000E+00  0.000E+00
   7  -6.594E-05 -1.049E-04  0.000E+00 -1.517E-04 -1.517E-04  0.000E+00 -1.049E-04 -6.594E-05  0.000E+00  0.000E+00  0.000E+00
   6  -5.432E-05 -8.125E-05 -1.049E-04 -1.133E-04 -1.049E-04 -8.125E-05 -5.432E-05  0.000E+00  0.000E+00  0.000E+00  0.000E+00
   5   0.000E+00 -5.432E-05 -6.594E-05 -6.594E-05 -5.432E-05  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits for General PT of TEST2
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |           | Sum[Denominator] |          |          |          |             |            |             |
[PERSENT]...|CORE2 | -9.519E+28|        -1.425E-01| 3.886E-03|-4.456E-03| 4.491E-02|   -2.358E-02|  -2.065E-02|    1.839E-01|
=PERSENT...Parameter General PT of TEST2    is -1.42515E-01 denominator  6.67952E+29 k-eff A  9.5337451E-01 F  8.3934021E-01
…
[PERSENT]...Axial plane     14 data for General PT of TEST2
              5          6          7          8          9         10         11         12         13         14         15
  15   0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.862E-04 -3.474E-04 -3.474E-04 -2.862E-04  0.000E+00
  14   0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.862E-04 -4.281E-04 -5.525E-04 -5.971E-04 -5.525E-04 -4.281E-04 -2.862E-04
  13   0.000E+00  0.000E+00  0.000E+00 -3.474E-04 -5.525E-04  0.000E+00 -7.994E-04 -7.994E-04  0.000E+00 -5.525E-04 -3.474E-04
  12   0.000E+00  0.000E+00 -3.474E-04 -5.971E-04 -7.994E-04  0.000E+00  0.000E+00  0.000E+00 -7.994E-04 -5.971E-04 -3.474E-04
  11   0.000E+00 -2.862E-04 -5.525E-04 -7.994E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -7.994E-04 -5.525E-04 -2.862E-04
  10   0.000E+00 -4.281E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -4.281E-04  0.000E+00
   9  -2.862E-04 -5.525E-04 -7.994E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -7.994E-04 -5.525E-04 -2.862E-04  0.000E+00
   8  -3.474E-04 -5.971E-04 -7.994E-04  0.000E+00  0.000E+00  0.000E+00 -7.994E-04 -5.971E-04 -3.474E-04  0.000E+00  0.000E+00
   7  -3.474E-04 -5.525E-04  0.000E+00 -7.994E-04 -7.994E-04  0.000E+00 -5.525E-04 -3.474E-04  0.000E+00  0.000E+00  0.000E+00
   6  -2.862E-04 -4.281E-04 -5.525E-04 -5.971E-04 -5.525E-04 -4.281E-04 -2.862E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
   5   0.000E+00 -2.862E-04 -3.474E-04 -3.474E-04 -2.862E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits/mass(kg) for General PT of TEST2
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |           | Sum[Denominator] |          |          |          |             |            |             |
[PERSENT]...|CORE2 | -8.360E+26|        -1.252E-03| 3.413E-05|-3.913E-05| 3.944E-04|   -2.070E-04|  -1.813E-04|    1.615E-03|
=PERSENT...Parameter General PT of TEST2    is -1.25154E-03 denominator  6.67952E+29 k-eff A  9.5337451E-01 F  8.3934021E-01
…
```

Figure 2-34. The PERSENT Worth/kg Excerpt for TEST2

2.2.6 *Verification of the Region and Area Output Tables*

To some degree, the mesh-wise and region-wise reactivity tables were checked in the preceding section. Because area-wise tables were not checked, this aspect is redone to verify both the region and area table output by manually computing it in EXCEL. This requires knowledge of which meshes go into which regions and which regions are part of each area. The benchmark specified by Figure 2-1 and Figure 2-3 is again used, but the DIF3D input is modified to include the area definitions shown at the top of Figure 2-35. The PERSENT perturbation input provided at the bottom of Figure 2-35 and was chosen to ensure many meshes would be impacted by the perturbation that would feed into the region and area calculations. This test case is benchmark 31 in the PERSENT distribution.

Figure 2-36 and Figure 2-37 provide the PERSENT calculated mesh-wise worth for the perturbation defined in Figure 2-35. Figure 2-38 provides the region and area-wise worth balance tables from the same PERSENT output. Because the regions selected in the perturbation for this model do not overlap radially, one can sum all the mesh-wise results over all axial planes to get the result shown in Table 2-17. In this table, the assembly positions associated with regions ROD1B, ROD2B, ROD3B, and ROD5B are colored to easily identify their positions. While tedious, it is a simple matter to verify that the data in Figure 2-36 and Figure 2-37 sum to the values in Table 2-17 and it is skipped here for brevity. The EXCEL calculated result is limited to four significant digits of accuracy as that is the precision of the mesh-wise values of PERSENT but 5 are given in the table.

The NOROD* to ROD perturbations in the PERSENT input impact the ROD1B, ROD2B, ROD3B, and ROD5B regions. The C1 to C2 perturbation impacts only the CORE1 region which fills all positions in the first three rings except the ROD1B location. The uncolored non-zero values in Table 2-17 correspond to the CORE1 results. The ROD4B region is not impacted. A review of the DIF3D input in Figure 2-3 shows that each of these control rod regions have a lower section, ROD1A as an example, followed by an upper section, ROD1B.

DIF3D Input Addition

```
07 RODA ROD1A ROD2A ROD3A ROD4A ROD5A
07 RODB ROD1B ROD2B ROD3B ROD4B ROD5B
07 C1C2 CORE1 CORE2
07 DOMN CORE1 CORE2 REFL  ABLAN RBLAN
07 DOMN ROD1A ROD2A ROD3A ROD4A ROD5A
07 DOMN ROD1B ROD2B ROD3B ROD4B ROD5B
```

PERSENT Input

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   dif3d.x
DIF3D_INPUT        dif3d_a.inp
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD1 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD2 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD3 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT NOROD5 ROD
ADJUST_ZONE   TEST2 GENERALIZED_PT C1     C2
PROBLEM_EDITS    TEST2 PRINT_BY_AREA PRINT_BY_REGION PRINT_BY_MESH PRINT_BALANCE
```

Figure 2-35. The Input Addition to DIF3D and PERSENT Perturbation Input

Looking at the ROD1B region result in Figure 2-38 is -4.009E-03 which matches the ROD1B result of -4.0086E-3 result in Table 2-17 within the round off error. The ROD2B region result in Figure 2-38 is -3.117E-02 which matches -7.7104E-3 + -5.1364E-3 + -1.8326E-2=-3.1174E-02 within the round off error. The ROD3B region result in Figure 2-38 is -3.480E-02 which matches -1.1996E-2 + -2.5365E-3 + -2.0270E-2=-3.4801E-2 within the round off error. The ROD5B region result in Figure 2-38 is -1.826E-04 which matches -1.7316E-4 + -1.1087E-5 + 1.5940E-6 =1.8265E-4 within the round off error. The CORE1 region result in Figure 2-38 is 7.628E-02 and summing all of the CORE1 related meshes in in Table 2-17 yields 7.6285E-02 which is again within the round off error.

For the areas, the RODB, C1C2, and DOMN are the only ones with non-zero values. The RODB area includes ROD1B, ROD2B, ROD3B, ROD4B, and ROD5B. The -7.017E-02 result from PERSENT matches the sum of region results -4.0086E-3 + -3.1174E-2 + -3.4801E-2 + −1.8265E-4= -7.0166E-2 from the hand calculated results above. It also matches the sum of the

region wise values from PERSENT of -4.009E-03 + -3.117E-02 + -3.480E-02 + -1.826E-04 = −7.0162E-2. The C1C2 result in Figure 2-38 is seen to identically match the reported region result for CORE1. The DOMN area consists of all regions in the domain and the 6.118E-03 result matches the parameter value result at the end of Figure 2-38 of 6.11787E-03 within round off error. The value can also be hand calculated from the region values as -4.009E-03 + -3.117E-02 + −3.480E-02 + -1.826E-04 + 7.628E-02 = 6.1184E-03. Note that the round off error prevents this result from matching the parameter result. One can also compute the DOMN result using the RODB and C1C2 areas -7.017E-02 + 7.628E-02 = 6.11E-03 where the round off error again restricts how accurate the result can be.

```
…
[PERSENT]...Axial plane      5 data for General PT of TEST2
              5           6           7           8           9          10          11          12          13          14          15
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.069E-04  2.232E-04  2.044E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.223E-04  2.452E-04  2.438E-04  2.183E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  2.021E-04  2.422E-04  0.000E+00  2.391E-04  1.967E-04  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  2.143E-04  2.366E-04  2.345E-04  2.089E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  1.912E-04  2.058E-04  1.862E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane      6 data for General PT of TEST2
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  3.484E-04  3.770E-04  3.434E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  3.757E-04  4.115E-04  4.088E-04  3.678E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  3.396E-04  4.058E-04  0.000E+00  3.998E-04  3.293E-04  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  3.597E-04  3.945E-04  3.905E-04  3.490E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  3.168E-04  3.420E-04  3.050E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane      7 data for General PT of TEST2
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  4.869E-04  5.264E-04  4.778E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.254E-04  5.737E-04  5.690E-04  5.122E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  4.737E-04  5.648E-04  0.000E+00  5.554E-04  4.571E-04  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  4.986E-04  5.463E-04  5.406E-04  4.828E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  4.321E-04  4.696E-04  4.177E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.958E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane      8 data for General PT of TEST2
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.881E-04  6.339E-04  5.724E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  6.354E-04  6.920E-04  6.847E-04  6.147E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  5.719E-04  6.809E-04  0.000E+00  6.677E-04  5.482E-04  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  5.983E-04  6.556E-04  6.488E-04  5.787E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  5.120E-04  5.592E-04  4.978E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -3.738E-03  0.000E+00  0.000E+00 -3.359E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane      9 data for General PT of TEST2
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  6.280E-04  6.731E-04  6.018E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  6.802E-04  7.387E-04  7.280E-04  6.500E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  6.125E-04  7.279E-04  0.000E+00  7.102E-04  5.802E-04  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  6.380E-04  6.988E-04  6.909E-04  6.145E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  5.414E-04  5.933E-04  5.283E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -3.713E-03  0.000E+00  0.000E+00 -3.554E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     10 data for General PT of TEST2
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -4.215E-03  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.980E-04  6.364E-04  5.603E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  6.506E-04  7.045E-04  6.906E-04  6.109E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  5.872E-04  6.964E-04  0.000E+00  6.745E-04  5.456E-04  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  6.107E-04  6.679E-04  6.589E-04  5.828E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  5.168E-04  5.661E-04  5.031E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -3.506E-03  0.000E+00  0.000E+00 -3.367E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     11 data for General PT of TEST2
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -3.236E-03  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.058E-04  5.360E-04  4.661E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.541E-04  5.990E-04  5.845E-04  5.114E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  5.025E-04  5.948E-04  0.000E+00  5.713E-04  4.535E-04 -3.308E-03  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  5.229E-04  5.709E-04  5.615E-04  4.923E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  4.425E-04  4.840E-04  4.287E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -2.967E-03  0.000E+00  0.000E+00 -2.837E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     12 data for General PT of TEST2
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.686E-03  0.000E+00  0.000E+00 -2.308E-03  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  3.705E-04  3.964E-04  3.450E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  4.124E-04  4.460E-04  4.346E-04  3.782E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00  0.000E+00  3.774E-04  4.452E-04  0.000E+00  4.249E-04  3.328E-04 -2.224E-03  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  3.932E-04  4.283E-04  4.201E-04  3.665E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
```

Figure 2-36. The PERSENT Mesh-Wise Worth Detail Output Excerpt of Planes 5 Through 12

From these hand calculations, the region and area tables are verified to be consistent with the expectation. For 60 degree and 120 degree periodic geometries, the PERSENT manual does indicate there is some nuance to computing these sums which is not verified here. While a more complicated problem could be generaated, there is no reason to believe that this test was not sufficient to ensure that all aspects of the area and region sum were working. In particular, the

areas contain regions that do and do not have perturbations and the result matches the expected result. This work satisifies the e) task of the category 2 work in Table 1-1.

```
[PERSENT]...Axial plane     13 data for General PT of TEST2
              5          6          7          8          9         10         11         12         13         14         15
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.510E-03  0.000E+00  0.000E+00 -1.383E-03  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.316E-04  2.503E-04  2.195E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.600E-04  2.760E-04  2.688E-04  2.399E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00 -1.591E-03  2.371E-04  2.762E-04 -2.492E-03  2.626E-04  2.118E-04 -1.330E-03  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  2.504E-04  2.662E-04  2.604E-04  2.336E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  2.152E-04  2.341E-04  2.074E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -1.344E-03  0.000E+00  0.000E+00 -1.279E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     14 data for General PT of TEST2
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.236E-04
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -6.642E-04  0.000E+00  0.000E+00 -6.094E-04  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.201E-04  1.300E-04  1.147E-04  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.342E-04  1.405E-04  1.371E-04  1.251E-04  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00 -6.726E-04  1.212E-04  1.406E-04 -1.073E-03  1.341E-04  1.111E-04 -5.960E-04  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  1.301E-04  1.362E-04  1.332E-04  1.223E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  1.133E-04  1.230E-04  1.094E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -6.078E-04  0.000E+00  0.000E+00 -5.804E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     15 data for General PT of TEST2
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -3.404E-05
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.973E-04  0.000E+00  0.000E+00 -1.763E-04  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  0.000E+00  0.000E+00 -1.972E-04  0.000E+00  0.000E+00 -3.194E-04  0.000E+00  0.000E+00 -1.797E-04  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -1.842E-04  0.000E+00  0.000E+00 -1.769E-04  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     16 data for General PT of TEST2
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.223E-05
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -6.322E-05  0.000E+00  0.000E+00 -5.508E-05  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10 -7.592E-06  0.000E+00 -6.127E-05  0.000E+00  0.000E+00 -1.001E-04  0.000E+00  0.000E+00 -5.815E-05  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -5.974E-05  0.000E+00  0.000E+00 -5.776E-05  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     17 data for General PT of TEST2
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -3.612E-06
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.662E-05  0.000E+00  0.000E+00 -1.414E-05  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10 -3.906E-06  0.000E+00 -1.543E-05  0.000E+00  0.000E+00 -2.565E-05  0.000E+00  0.000E+00 -1.540E-05  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -1.584E-05  0.000E+00  0.000E+00 -1.538E-05  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
[PERSENT]...Axial plane     18 data for General PT of TEST2
    15  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  3.171E-07
    14  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    13  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  9.003E-07  0.000E+00  0.000E+00  9.741E-07  0.000E+00  0.000E+00
    12  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    11  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
    10  4.107E-07  0.000E+00  1.035E-06  0.000E+00  0.000E+00  1.537E-06  0.000E+00  0.000E+00  8.243E-07  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
```

Figure 2-37. The PERSENT Mesh-Wise Worth Detail Output Excerpt of Planes 13 Through 18

```
[PERSENT]...Region edits for General PT of TEST2
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  ||   n,2n   |
[PERSENT]...|      |           | Sum[Denominator] |           |          |           |             |              ||          |
[PERSENT]...|REFL  |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ABLAN |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|RBLAN |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|CORE1 |  3.570E+28|          7.628E-02|-1.010E-03| 2.750E-03|-2.686E-02|    1.633E-02|   1.461E-02|   -9.968E-02|| 7.137E-05|
[PERSENT]...|CORE2 |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD1A |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD2A |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD3A |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD4A |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD5A |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD1B | -1.876E+27|         -4.009E-03| 1.388E-03|-5.002E-03| 0.000E+00|   -3.282E-03|  -2.888E-03|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD2B | -1.459E+28|         -3.117E-02| 4.888E-03|-3.434E-02| 0.000E+00|   -2.213E-02|  -2.041E-02|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD3B | -1.629E+28|         -3.480E-02| 5.165E-03|-3.807E-02| 0.000E+00|   -2.462E-02|  -2.272E-02|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD4B |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|ROD5B | -8.546E+25|         -1.826E-04| 3.303E-04|-4.627E-04| 0.000E+00|   -2.370E-04|  -1.868E-04|    0.000E+00|| 0.000E+00|
[PERSENT]...Area edits for General PT of TEST2
[PERSENT]...| Area | Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  ||   n,2n   |
[PERSENT]...|      |           | Sum[Denominator] |           |          |           |             |              ||          |
[PERSENT]...|RODA  |  0.000E+00|          0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|| 0.000E+00|
[PERSENT]...|RODB  | -3.283E+28|         -7.017E-02| 1.177E-02|-7.787E-02| 0.000E+00|   -5.027E-02|  -4.620E-02|    0.000E+00|| 0.000E+00|
[PERSENT]...|C1C2  |  3.570E+28|          7.628E-02|-1.010E-03| 2.750E-03|-2.686E-02|    1.633E-02|   1.461E-02|   -9.968E-02|| 7.137E-05|
[PERSENT]...|DOMN  |  2.863E+27|          6.118E-03| 1.076E-02|-7.512E-02|-2.686E-02|   -3.394E-02|  -3.159E-02|   -9.968E-02|| 7.137E-05|
=PERSENT...Parameter General PT of TEST2             is  6.11787E-03 denominator  4.67949E+29 k-eff A  8.9452702E-01 F  8.9944482E-01
```

Figure 2-38. The PERSENT Region and Area Worth Output Excerpt

Table 2-17. Sum of Mesh-wise PERSENT Result Over All Axial Planes

Row	5	7	8	9	10	11	12	13	15
15									-1.7316E-4
14									
13					-5.1364E-3			-1.1996E-2	
12					4.0843E-3	4.3827E-3	3.9054E-3		
11				4.4503E-3	4.8271E-3	4.7499E-3	4.2285E-3		
10	-1.1087E-5	-2.5365E-3	4.0252E-3	4.7748E-3	-4.0086E-3	4.6396E-3	3.7663E-3	-7.7104E-3	
9			4.2162E-3	4.6013E-3	4.5394E-3	4.0314E-3			
8			3.6153E-3	3.9417E-3	3.5058E-3				
7		-1.8326E-2			-2.0270E-2				
6									
5					1.5940E-6				
	ROD1B	ROD2B	ROD3B	ROD5B	CORE1				

2.3 First Order Perturbation Verification

In the preceding section, the exact perturbation details were verified and thus the category 2 verification work was completed. The category 3 verification work covered in this section is focused on the first order perturbation option of PERSENT. Because the exact perturbation option is exact, it should be clear that the first order perturbation theory option is not exact, but an approximation of the exact perturbation result. The PERSENT manual indicates that the first order perturbation theory option can only match the exact perturbation result if the total perturbation is small. In this regard, PERSENT will alter the user provided perturbation to put it in the range where first order perturbation is known to match the exact perturbation. Given the calculated first order perturbation worth of the altered user perturbation, PERSENT will scale that result back to the magnitude desired by the user.

From this basic description, there are two aspects to verify. First, the first order perturbation theory result should identically produce the exact perturbation result for a "small" perturbation. Second, PERSENT scales the user provided perturbation both up and down. The first aspect is very easy to verify as one just needs to compare the exact perturbation theory result with the first order perturbation result as the user perturbation is decreased. The second aspect is also very easy given the first order perturbation result is known.

The benchmark specified earlier in Figure 2-1 and Figure 2-3 is used for this verification work. Two separate tests are considered for perturbing zones NOROD3 and C1 in the original input. For NOROD3, a control rod material is mixed into the non-control-rod material as is outlined in Table 2-18 which provides the atom densities of the mixed materials. As can be seen, the first control rod perturbation (RODTEST1) is mostly composed of the NOROD material (99.99%) while the last material only contains a modest amount (10%) of the control rod material. The C1 perturbation is setup similarly as seen in Table 2-19. In the C1 perturbation, only the U238 and PU239 concentrations are adjusted between the perturbed states.

Table 2-18. Control Rod Perturbation for First Order Verification

			RODTEST1	RODTEST2	RODTEST3	RODTEST4	RODTEST5
	NOROD	ROD	0.0001	0.0005	0.001	0.005	0.100
NA	0.022	0.0104	2.19988E-02	2.19942E-02	2.19884E-02	2.19420E-02	2.08400E-02
FE		0.0181	1.81000E-06	9.05000E-06	1.81000E-05	9.05000E-05	1.81000E-03
O-16		0.0149	1.49000E-06	7.45000E-06	1.49000E-05	7.45000E-05	1.49000E-03
B-10		0.0090	9.00000E-07	4.50000E-06	9.00000E-06	4.50000E-05	9.00000E-04
C		0.0412	4.12000E-06	2.06000E-05	4.12000E-05	2.06000E-04	4.12000E-03

Table 2-19. Core C1 Perturbation for First Order Verification

			C1TEST1	C1TEST2	C1TEST3	C1TEST4	C1TEST5
	C1	MOD	0.00001	0.0001	0.0005	0.0010	0.1000
NA	0.0104	0.0104	1.04000E-02	1.04000E-02	1.04000E-02	1.04000E-02	1.04000E-02
O-16	0.0149	0.0149	1.49000E-02	1.49000E-02	1.49000E-02	1.49000E-02	1.49000E-02
FE	0.0181	0.0181	1.81000E-02	1.81000E-02	1.81000E-02	1.81000E-02	1.81000E-02
U238	0.0064	0.005	6.39999E-03	6.39986E-03	6.39930E-03	6.39860E-03	6.26000E-03
PU239	0.0011	0.0025	1.10001E-03	1.10014E-03	1.10070E-03	1.10140E-03	1.24000E-03

The PERSENT input for this set of perturbations is given in Figure 2-39. Because PERSENT performs the calculations in the sequence that they are entered and it provides the problem name for each case, the output for each test is easy to identify and all tests are run in a single PERSENT input. The PERSENT test case is benchmark 26 in the PERSENT distribution and benchmark 48 is a separate test of the base DIF3D model.

The worth results for the control rod is given in Table 2-20. The results are given in pcm noting that accuracy below 0.01 pcm is typically rather unreliable for exact perturbation calculations. In Table 2-20, the results are organized by row according to the mixing fraction from Table 2-18. The first column is the exact perturbation PERSENT result from RODTEST1 to RODTEST5.

```
…
NEW_ZONE ROD01 NA 2.19988E-02 FE 1.81000E-06 O-16 1.49000E-06 B-10 9.00000E-07 C 4.12000E-06
NEW_ZONE ROD02 NA 2.19942E-02 FE 9.05000E-06 O-16 7.45000E-06 B-10 4.50000E-06 C 2.06000E-05
NEW_ZONE ROD03 NA 2.19884E-02 FE 1.81000E-05 O-16 1.49000E-05 B-10 9.00000E-06 C 4.12000E-05
NEW_ZONE ROD04 NA 2.19420E-02 FE 9.05000E-05 O-16 7.45000E-05 B-10 4.50000E-05 C 2.06000E-04
NEW_ZONE ROD05 NA 2.08400E-02 FE 1.81000E-03 O-16 1.49000E-03 B-10 9.00000E-04 C 4.12000E-03
NEW_ZONE  C1M01 NA 1.04000E-02 O-16 1.49000E-02 FE 1.81000E-02 U238 6.39999E-03 PU239 1.10001E-03
NEW_ZONE  C1M02 NA 1.04000E-02 O-16 1.49000E-02 FE 1.81000E-02 U238 6.39986E-03 PU239 1.10014E-03
NEW_ZONE  C1M03 NA 1.04000E-02 O-16 1.49000E-02 FE 1.81000E-02 U238 6.39930E-03 PU239 1.10070E-03
NEW_ZONE  C1M04 NA 1.04000E-02 O-16 1.49000E-02 FE 1.81000E-02 U238 6.39860E-03 PU239 1.10140E-03
NEW_ZONE  C1M05 NA 1.04000E-02 O-16 1.49000E-02 FE 1.81000E-02 U238 6.26000E-03 PU239 1.24000E-03
ADJUST_ZONE      RODTEST1 GENERALIZED_PT NOROD3 ROD01
ADJUST_ZONE      RODTEST2 GENERALIZED_PT NOROD3 ROD02
ADJUST_ZONE      RODTEST3 GENERALIZED_PT NOROD3 ROD03
ADJUST_ZONE      RODTEST4 GENERALIZED_PT NOROD3 ROD04
ADJUST_ZONE      RODTEST5 GENERALIZED_PT NOROD3 ROD05
PROBLEM_EDITS    RODTEST1 PRINT_BY_MESH PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    RODTEST2 PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    RODTEST3 PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    RODTEST4 PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    RODTEST5 PRINT_BY_REGION PRINT_BALANCE

ADJUST_ZONE      FO_RODTEST1 FIRST_ORDER_PT NOROD3 ROD01
ADJUST_ZONE      FO_RODTEST2 FIRST_ORDER_PT NOROD3 ROD02
ADJUST_ZONE      FO_RODTEST3 FIRST_ORDER_PT NOROD3 ROD03
ADJUST_ZONE      FO_RODTEST4 FIRST_ORDER_PT NOROD3 ROD04
ADJUST_ZONE      FO_RODTEST5 FIRST_ORDER_PT NOROD3 ROD05
PROBLEM_EDITS    FO_RODTEST1 PRINT_BY_MESH PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_RODTEST2 PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_RODTEST3 PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_RODTEST4 PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_RODTEST5 PRINT_BY_REGION PRINT_BALANCE

ADJUST_ZONE      C1TEST1 GENERALIZED_PT C1 C1M01
ADJUST_ZONE      C1TEST2 GENERALIZED_PT C1 C1M02
ADJUST_ZONE      C1TEST3 GENERALIZED_PT C1 C1M03
ADJUST_ZONE      C1TEST4 GENERALIZED_PT C1 C1M04
ADJUST_ZONE      C1TEST5 GENERALIZED_PT C1 C1M05
PROBLEM_EDITS    C1TEST1 PRINT_BY_MESH PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    C1TEST2 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    C1TEST3 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    C1TEST4 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    C1TEST5 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE

ADJUST_ZONE      FO_C1TEST1 FIRST_ORDER_PT C1 C1M01
ADJUST_ZONE      FO_C1TEST2 FIRST_ORDER_PT C1 C1M02
ADJUST_ZONE      FO_C1TEST3 FIRST_ORDER_PT C1 C1M03
ADJUST_ZONE      FO_C1TEST4 FIRST_ORDER_PT C1 C1M04
ADJUST_ZONE      FO_C1TEST5 FIRST_ORDER_PT C1 C1M05
PROBLEM_EDITS    FO_C1TEST1 PRINT_BY_MESH PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_C1TEST2 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_C1TEST3 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_C1TEST4 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
PROBLEM_EDITS    FO_C1TEST5 PRINT_BY_MASS PRINT_BY_REGION PRINT_BALANCE
…
```

Figure 2-39. The PERSENT Input for First Order Perturbation Verification

The second column in Table 2-20 is the PERSENT reported first order perturbation results for FO_RODTEST1 to FO_RODTEST5. The fourth column (Rescaled Exact) is the result when the first exact perturbation result (-0.520708 pcm) is manually scaled to the correct magnitude of the perturbation. As an example, -2.60354 = -0.520708*0.0005/0.0001. The last column (Rescaled First Order) takes the first order result from the third column (-0.520735) and scales it in a similar manner to that done in the fourth column -2.60368 = -0.520735*0.0005/0.0001.

Table 2-20. Perturbation Worth Results (pcm) for the Control Rod Perturbation

	Exact	First Order	Rescaled Exact	Rescaled First Order
0.0001	-0.520708	-0.520735		
0.0005	-2.60299	-2.60366	-2.60354	-2.60368
0.0010	-5.20463	-5.20733	-5.20708	-5.20735
0.0050	-25.9696	-26.0366	-26.0354	-26.0368
0.1000	-495.288	-520.732	-520.708	-520.735

As can be seen, the exact perturbation result and the first order perturbation result are very similar for the 0.0001, 0.0005, and 0.0010 perturbations. As the perturbation becomes larger, one can see a clear distinction between the exact and first order result with the largest difference at the 0.1 perturbation. As stated, the essence of the first order perturbation approach is to scale a given perturbation to and from the small perturbation range. A comparison between the third column (First Order) and fourth column (Rescaled Exact) results shows very similar predicted results even up to the largest perturbation of 0.1. The good agreement in the results for columns 3 through 5 should make it clear that PERSENT is correctly scaling each user perturbation down to the ~1 pcm range and then scaling it back up to the user specified magnitude assuming linear extrapolation. The fact that the PERSENT first order perturbation result for the smallest perturbation reproduced the first order values (i.e. column 5 is similar to column 3) indicates that PERSENT is correctly obtaining the first order perturbation result on this test case.

Table 2-21 provides the C1 core perturbation worth results along with the manually scaled results similar to that done for Table 2-20. From inspection of the first order and exact perturbation results, it should be clear that the C1 perturbation is more linear than the control rod perturbation result of Table 2-20 as the first order perturbation results from PERSENT are nearly identical to the exact perturbation up to 0.001 with a much smaller error on the 0.1 perturbation than that seen in Table 2-20. This is not a surprise given the relative importance of the two regions with respect to the eigenvalue.

Table 2-21. Perturbation Worth Results (pcm) for the Core C1 Perturbation

	Exact	First Order	Rescaled Exact	Rescaled First Order		
0.00001	0.224393	0.224393			0.224929	0.224878
0.00010	2.24927	2.24929	2.24393	2.24393		2.24878
0.00050	11.2434	11.2439	11.2196	11.2196	11.2465	
0.00100	22.4859	22.4877	22.4393	22.4393	22.4929	22.4878
0.10000	2228.52	2248.70	2243.93	2243.93	2249.29	2248.78

The rescaled first order results in Table 2-21 were generated taking the first three perturbation results from the first order routine. Because the exact (second column) and first order perturbation results (second and third column 0.224393 result) are virtually identical at the 0.00001 perturbation, it should not be a surprise that the fourth column (Rescaled Exact) identically matches the results in the fifth column (First column of results for Rescaled First Order). The additional two columns (6^{th} and 7^{th}) of the First order case were done to demonstrate that the perturbation worth does not strictly have to be less than 1 pcm to guarantee a good result when using the first order extrapolation assumption.

In the PERSENT manual, it states that it will not scale the user perturbation when the estimated exact perturbation worth is less than 1 pcm. Instead, PERSENT will simply use the first order perturbation equation which will be effectively exact if the perturbation is indeed small as is the case for the 0.00001 perturbation. It is worth noting that the PERSENT methodology for first order result is more consistent with using a larger reactivity worth in this demonstrated case (the 2248.70 result in column 3 is more consistent with 2249.29 in column 6 and 2248.78 in column 7 than with 2243.93 result in column 5). This would generally indicate that the built-in methodology is likely

restricted to 3 digits of accuracy on the reactivity coefficient which is likely beyond the precision of accuracy of the point kinetics methodology.

In an attempt to expose any issues with convergence, the Omega acceleration was disabled and the PERSENT calculation was redone. This should cause a different path to convergence and thus, to some degree, different error in the higher order space-angle moments of the solution. The DIF3D eigenvalue results for all of the exact perturbation cases along with the base state forward and adjoint eigenvalues are summarized in Table 2-22. These are the reported eigenvalues in the PERSENT output and thus there is some amount of truncation error present in all of them. The worth calculation for each perturbation problem of interest is also provided using those eigenvalues along with the PERSENT reported exact perturbation worth of each case. As can be seen, the PERSENT calculated worth is identical for all of the perturbations while the exact calculated result is slightly different from the PERSENT value. The worth computed using the two sets of eigenvalues is also different indicating the magnitude of importance of the residual eigenvalue convergence. As was identified earlier, these errors are not unexpected and are again of little concern for the results shown here.

Table 2-22. Core C1 Perturbation Eigenvalue Results

	With Omega	Worth (pcm)	PERSENT Exact	No Omega	Worth (pcm)	PERSENT Exact
Adjoint	0.95337 45			0.95337 43		
Forward	0.95337 44			0.95337 43		
0.00001	0.95337 59	0.222241	0.224393	0.95337 58	0.222241	0.224393
0.00010	0.95339 48	2.24877	2.24927	0.95339 48	2.24877	2.24927
0.00050	0.95347 66	11.2451	11.2434	0.95347 65	11.2385	11.2434
0.00100	0.95357 88	22.4877	22.4859	0.95357 87	22.4811	22.4859
0.10000	0.97406 87	2228.42	2228.52	0.97406 86	2228.42	2228.52

The preceding results confirm that PERSENT is correctly scaling the user perturbation to the range where the first order approximation is accurate. It also demonstrates that PERSENT correctly scales that result back to the magnitude requested by the user. Further the first order perturbation results do not reproduce the exact perturbation results unless the perturbation itself is small which is the expected behavior. In the remainder of this section, the detailed mesh wise results from the first order perturbation theory output are verified.

The control rod test only impacts three x-y mesh positions for axial planes 7 to 18. In Figure 2-40, the axial plane data for planes 7 through 18 for the exact perturbation and three first order perturbation results are collected together for just one particular x-y position (J=7 and I=10). The exact and first order perturbation result for the 0.0001 magnitude perturbation are included along with the first order ones for 0.0005 and 0.10. (Note that PRINT_BY_MESH was only enabled for these cases in the PERSENT input in Figure 2-39).

Comparison of the 0.0001 exact and first order perturbation mesh wise results shows that only the fourth significant digit changes for some of the reported values. The sum of the displayed

results will not equal the total worth as there are two other x-y positions impacted by the perturbation, but the sum should also scale.

Exact Perturbation Theory 0.0001

	1	2	3	4	5	6	7	8	9	10
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.604E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.680E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.285E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.285E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.680E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.604E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.299E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	**-1.083E-07**
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.099E-08
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-8.469E-09
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.980E-09
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	**8.950E-10**

First order 0.0001

7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.604E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.681E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.286E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.286E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.681E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.604E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.299E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.083E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.099E-08
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-8.468E-09
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.979E-09
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	8.954E-10

First order 0.0005

7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.802E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.340E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.643E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.643E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.340E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.802E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.149E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.416E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.549E-07
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.233E-08
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-9.894E-09
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.478E-09

First order 0.10

7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.604E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.681E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.286E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-5.286E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-4.681E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.604E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-2.299E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.083E-04
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-3.098E-05
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-8.467E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-1.979E-06
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	8.955E-07

Figure 2-40. Mesh-wise Control Rod Worth Perturbation Output Excerpt

Using the same scaling approach as was done for the total worth in Table 2-20 and Table 2-21, the exact and first order perturbation results were scaled to the magnitude of each other. Instead of reporting those scaled answers, as was done in Table 2-20 and Table 2-21, only the error between the expected result and the PERSENT reported value is provided in Table 2-23. Because the mesh-wise values in the PERSENT output only provide 4 significant digits of accuracy, the accuracy of the scaling should not be expected to be worse than 0.1% and the results show the error is well below for most meshes this with a maximum of -0.067%.

The results in Table 2-23 include the error in the expected result when the three first order solutions (columns 3, 4, and 5) are scaled to the exact perturbation result for the 0.0001 modification. Also included is the error in the expected result when the 0.1 first order perturbation

result is scaled to the 0.0005 magnitude (5th column). From the results shown, one can conclude that the first order perturbation results are somewhat more consistent (less error) with each other than with the exact perturbation result, but it is difficult to eliminate the truncation error contribution to these results.

Table 2-23. Mesh-wise Control Rod Worth Error Results

Axial Plane	Exact Perturbation Worth 0.0001	Error of Scaled First Order Result with Exact 0.0001 Result			Error of Scaled First Order 0.0005 Result with First Order 0.1 Result
		0.0001	0.0005	0.10	
7	-3.604E-07	0.000%	0.000%	0.000%	0.000%
8	-4.680E-07	0.021%	0.000%	0.021%	0.021%
9	-5.285E-07	0.019%	0.019%	0.019%	0.000%
10	-5.285E-07	0.019%	0.019%	0.019%	0.000%
11	-4.680E-07	0.021%	0.000%	0.021%	0.021%
12	-3.604E-07	0.000%	0.000%	0.000%	0.000%
13	-2.299E-07	0.000%	-0.043%	0.000%	0.044%
14	**-1.083E-07**	0.000%	0.018%	0.000%	-0.018%
15	-3.099E-08	0.000%	-0.032%	-0.032%	0.000%
16	-8.469E-09	-0.012%	-0.035%	-0.024%	0.012%
17	-1.980E-09	-0.051%	-0.061%	-0.051%	0.010%
18	**8.950E-10**	0.045%	0.067%	0.056%	-0.011%
Sum	-3.093E-06	0.013%	0.003%	0.012%	0.009%

From Figure 2-40, the exact perturbation worth of plane 14 is **0.01083** pcm while the worth on plane 18 is **0.0000895** pcm. In theory, the first order perturbation result should yield an identical result to the exact perturbation in each mesh, but from Figure 2-40, one can see that the error increases as the total worth of a given mesh decreases. Using the first order perturbation result from 0.0001 to compute the scaling to the 0.0005 and 0.10 levels does not appreciably improve the accuracy compared with using the exact perturbation worth. As was the case with the total worth issues, one can attribute these problems to the inaccurate nature of the flux vectors for the small perturbation being applied. Given that PERSENT is properly scaling all of the other first order perturbations to a magnitude greater than the 0.0001 perturbation result, we can conclude that PERSENT is more reliable at determining the scaling than the manual approach taken here (i.e. selection of 0.0001, 0.0005, 0.001, 0.005 and 0.10). Once again, the user should not provide PERSENT with a small perturbation worth, << 1 pcm, and expect the results from the perturbation equation to be highly accurate as there are limits on convergence of the eigenvalue and flux solution.

The C1 core perturbation impacts a much larger number of meshes in the x-y plane and impacts axial planes 5 through 14. As was done for the control rod perturbation, only a single line of the mesh-wise output was chosen and was collected for all axial planes in Figure 2-41. The results of the exact perturbation result for the 0.0001 modification and the first order perturbation results for

the 0.0001 and 0.1 modifications are provided in Figure 2-41. Table 2-24 provides the error in the scaled 0.1 values to the 0.0001 level which again are limited by the 4 significant digits of output in the PERSENT output.

Exact Perturbation Theory 0.0001

```
[PERSENT]...Axial plane      5 data for General PT of C1TEST2
        1 ...       6         7         8         9        10        11        12
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  5.142E-08  5.542E-08  5.542E-08  5.142E-08
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  9.100E-08  9.744E-08  9.744E-08  9.100E-08
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.321E-07  1.412E-07  1.412E-07  1.321E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.657E-07  1.770E-07  1.770E-07  1.657E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.657E-07  1.770E-07  1.770E-07  1.657E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.321E-07  1.412E-07  1.412E-07  1.321E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  9.100E-08  9.744E-08  9.744E-08  9.100E-08
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  5.142E-08  5.542E-08  5.542E-08  5.142E-08
```

First order 0.0001

```
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  5.142E-08  5.542E-08  5.542E-08  5.142E-08
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  9.100E-08  9.744E-08  9.744E-08  9.100E-08
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.321E-07  1.412E-07  1.412E-07  1.321E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.657E-07  1.770E-07  1.770E-07  1.657E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.657E-07  1.770E-07  1.770E-07  1.657E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.321E-07  1.412E-07  1.412E-07  1.321E-07
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  9.100E-08  9.744E-08  9.744E-08  9.100E-08
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  5.142E-08  5.542E-08  5.542E-08  5.142E-08
```

First order 0.10

```
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  5.140E-05  5.540E-05  5.540E-05  5.140E-05
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  9.098E-05  9.742E-05  9.742E-05  9.098E-05
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.320E-04  1.411E-04  1.411E-04  1.320E-04
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.656E-04  1.770E-04  1.770E-04  1.656E-04
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.844E-04  1.970E-04  1.970E-04  1.844E-04
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.844E-04  1.970E-04  1.970E-04  1.844E-04
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.656E-04  1.770E-04  1.770E-04  1.656E-04
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  1.320E-04  1.411E-04  1.411E-04  1.320E-04
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  9.098E-05  9.742E-05  9.742E-05  9.098E-05
11  0.000E+00   0.000E+00  0.000E+00  0.000E+00  5.140E-05  5.540E-05  5.540E-05  5.140E-05
```

Figure 2-41. Mesh-wise C1 Core Worth Perturbation Output Excerpt

Table 2-24. Mesh-wise C1 Worth Error Results

Axial Plane	Exact 0.0001 Perturbation Worth				Error in First Order 0.1 Scaled to Exact 0.0001			
	9	10	11	12	9	10	11	12
5	5.142E-08	5.542E-08	5.542E-08	5.142E-08	0.039%	0.036%	0.036%	0.039%
6	9.100E-08	9.744E-08	9.744E-08	9.100E-08	0.022%	0.021%	0.021%	0.022%
7	1.321E-07	1.412E-07	1.412E-07	1.321E-07	0.076%	0.071%	0.071%	0.076%
8	1.657E-07	1.770E-07	1.770E-07	1.657E-07	0.060%	0.000%	0.000%	0.060%
9	1.845E-07	1.971E-07	1.971E-07	1.845E-07	0.054%	0.051%	0.051%	0.054%
10	1.845E-07	1.971E-07	1.971E-07	1.845E-07	0.054%	0.051%	0.051%	0.054%
11	1.657E-07	1.770E-07	1.770E-07	1.657E-07	0.060%	0.000%	0.000%	0.060%
12	1.321E-07	1.412E-07	1.412E-07	1.321E-07	0.076%	0.071%	0.071%	0.076%
13	9.100E-08	9.744E-08	9.744E-08	9.100E-08	0.022%	0.021%	0.021%	0.022%
14	5.142E-08	5.542E-08	5.542E-08	5.142E-08	0.039%	0.036%	0.036%	0.039%
Sum	1.249E-06	1.336E-06	1.336E-06	1.249E-06	0.054%	0.036%	0.036%	0.054%

A quick review of the 0.0001 results in Figure 2-41 show that the first order and exact perturbation are identical for all values. This only occurs because of the limited precision in the mesh-wise

output rather then the results being exactly the same. Since the scaling between the exact 0.0001 and 0.10 first order perturbation result is 1000, the 0.10 results can be visually compared in Figure 2-41 for accuracy but Table 2-24 is provided to confirm the accuracy of the scaled results. As seen, the errors are small and consistent with the results for the control rod test in Table 2-23. The last aspect to verify is that the mass and the worth/kg results are correct for the first order perturbation result. Since the exact perturbation should end up with the identical mass calculation and the worth/kg for small perturbations, a direct comparison of the output is all that is required for this verification. Figure 2-42 provides the plane 9 excerpt of output for the exact and first order 0.0001 perturbation.

Exact Perturbation Theory 0.0001

```
[PERSENT]...Axial plane      9 data for mass(kg) change for C1TEST2
               1 ...         6           7           8           9          10          11          12
    12  0.000E+00    0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07
    11  0.000E+00    0.000E+00  0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07  2.900E-07
    10  0.000E+00    0.000E+00  0.000E+00  2.900E-07  2.900E-07  0.000E+00  2.900E-07  2.900E-07
     9  0.000E+00    0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07  2.900E-07  0.000E+00
     8  0.000E+00    0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07  0.000E+00  0.000E+00
 [PERSENT]...Axial plane      9 data for General PT of C1TEST2   (worth)
               1 ...         6           7           8           9          10          11          12
    12  0.000E+00    0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.717E-07  1.845E-07  1.717E-07
    11  0.000E+00    0.000E+00  0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07
    10  0.000E+00    0.000E+00  0.000E+00  1.717E-07  1.971E-07  0.000E+00  1.971E-07  1.717E-07
     9  0.000E+00    0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07  0.000E+00
     8  0.000E+00    0.000E+00  0.000E+00  1.717E-07  1.845E-07  1.717E-07  0.000E+00  0.000E+00
[PERSENT]...Axial plane      9 data for General PT of C1TEST2    (worth/kg)
               1 ...         6           7           8           9          10          11          12
    12  0.000E+00    0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.921E-01  6.361E-01  5.921E-01
    11  0.000E+00    0.000E+00  0.000E+00  0.000E+00  6.361E-01  6.796E-01  6.796E-01  6.361E-01
    10  0.000E+00    0.000E+00  0.000E+00  5.921E-01  6.796E-01  0.000E+00  6.796E-01  5.921E-01
     9  0.000E+00    0.000E+00  0.000E+00  6.361E-01  6.796E-01  6.796E-01  6.361E-01  0.000E+00
     8  0.000E+00    0.000E+00  0.000E+00  5.921E-01  6.361E-01  5.921E-01  0.000E+00  0.000E+00
```

First order 0.0001

```
[PERSENT]...Axial plane      9 data for mass(kg) change for FO_C1TEST2
               1 ...         6           7           8           9          10          11          12
    12  0.000E+00    0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07
    11  0.000E+00    0.000E+00  0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07  2.900E-07
    10  0.000E+00    0.000E+00  0.000E+00  2.900E-07  2.900E-07  0.000E+00  2.900E-07  2.900E-07
     9  0.000E+00    0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07  2.900E-07  0.000E+00
     8  0.000E+00    0.000E+00  0.000E+00  2.900E-07  2.900E-07  2.900E-07  0.000E+00  0.000E+00
[PERSENT]...Axial plane      9 data for First O PT of FO_C1TEST2 (worth)
               1 ...         6           7           8           9          10          11          12
    12  0.000E+00    0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.717E-07  1.845E-07  1.717E-07
    11  0.000E+00    0.000E+00  0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07
    10  0.000E+00    0.000E+00  0.000E+00  1.717E-07  1.971E-07  0.000E+00  1.971E-07  1.717E-07
     9  0.000E+00    0.000E+00  0.000E+00  1.845E-07  1.971E-07  1.971E-07  1.845E-07  0.000E+00
     8  0.000E+00    0.000E+00  0.000E+00  1.717E-07  1.845E-07  1.717E-07  0.000E+00  0.000E+00
[PERSENT]...Axial plane      9 data for First O PT of FO_C1TEST2 (worth/kg)
               1 ...         6           7           8           9          10          11          12
    12  0.000E+00    0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.921E-01  6.361E-01  5.921E-01
    11  0.000E+00    0.000E+00  0.000E+00  0.000E+00  6.361E-01  6.796E-01  6.796E-01  6.361E-01
    10  0.000E+00    0.000E+00  0.000E+00  5.921E-01  6.796E-01  0.000E+00  6.796E-01  5.921E-01
     9  0.000E+00    0.000E+00  0.000E+00  6.361E-01  6.796E-01  6.796E-01  6.361E-01  0.000E+00
     8  0.000E+00    0.000E+00  0.000E+00  5.921E-01  6.361E-01  5.921E-01  0.000E+00  0.000E+00
```

Exact 0.10

```
[PERSENT]...Region edits for mass(kg) change for C1TEST5
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|ABLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|RBLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |  0.000E+00|         3.279E-02|
```

First order 0.10

```
 [PERSENT]...Region edits for mass(kg) change for FO_C1TEST5
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|ABLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|RBLAN |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |  0.000E+00|         3.279E-02|
```

Figure 2-42. Mesh-wise C1 Core Mass and Worth/kg Excerpt

In each segment of output, the mass output excerpt for the plane is provided followed by the worth and then worth/kg. Also included at the bottom are the region edit summary table produced by

PERSENT of the mass change for the exact and first order perturbation with the 0.1 modification. Looking at the mesh-wise mass output, one finds that the exact perturbation and first order perturbation are identical. This is not a surprise since the perturbation itself is identical and the mass calculation is independent of the worth. The mesh-wise worth results appear identical, as was the case with Figure 2-41, because of the limited precision on the PERSENT output. Finally, the worth/kg mesh-wise results also appear identical which are precision limited. Looking at the region-wise output edit, the total mass change is identical which is expected as the perturbation itself is identical. The worth/kg result is also identical but not shown for brevity.

The preceding control rod and C1 core perturbation results indicate that PERSENT will correctly obtain the first order perturbation worth, within 3 significant digits, given that the provided perturbation is non-trivial. The first order perturbation is an approximation and should never be expected to exactly reproduce the exact perturbation result. If the perturbation itself is relatively linear, the first order perturbation approximation can be very accurate over a large perturbation range as observed with the C1 core perturbation results. The preceding results complete the a), b), and c) tasks of category 3 verification work in Table 1-1.

2.4 First Order Bowing Worth Perturbation Verification

The bowing worth perturbation methodology used in PERSENT is rather difficult to verify because of the underlying geometry issues. One major aspect of difficulty is defining multi-group cross sections for the heterogeneous geometry that are consistent with the multi-group cross sections generated for the homogeneous geometry. It is not hard to show that reinterpretating the homogeneous geometry cross sections for the heterogeneous geometry will lead to 2-3% error in k_{eff} when using multi-group MCNP compared with the original homogeneous result for conventional cross sections. It should be noted that the homogeneous result typically agrees well with the continuous energy MCNP solution and measured values in experiments. It is hard to justify that a multi-group MCNP model can produce a valid reference solution for the bowing worth perturbation methodology in PERSENT for perturbation magnitudes of ~0.02% when it has a fundamental 3% error.

The easiest way to avoid this problem is to use manufactured cross sections that DIF3D can tackle in both heterogeneous and homogeneous models. Given one can define cross sections for a heterogeneous problem that can be solved with DIF3D, one should be able to construct region-wise cross sections by flux weighting the heterogeneous cross sections for a homogeneous problem representation. The accuracy of this approach is of course limited to the size of the region that the cross section data is being collapsed over. Regardless, there will always be some degree of mismatch between the homogeneous problem and the heterogeneous problem that will prevent the homogeneous problem from obtaining an equivalent answer to the heterogeneous one.

To make the verification possible, a one-group cross section set was constructed for testing the bowing worth computation. Because a heterogeneous and homogeneous equivalent using just DIF3D can only be defined on a Cartesian geometry, a 3D Cartesian geometry problem was constructed, the details of which are shown in Figure 2-43. The PERSENT test case is benchmark 30 in the PERSENT distribution. The left two pictures show the homogeneous geometry which has three material regions and a pitch of 10 cm. The right two pictures have six material regions and a pitch of 10 cm. PERSENT has a safety check in place which prevents the duct pitch to be $\leq$ 90% or $\geq$ 99.5% of the assembly pitch itself (10 cm). The duct pitch was selected as 9.1 cm.

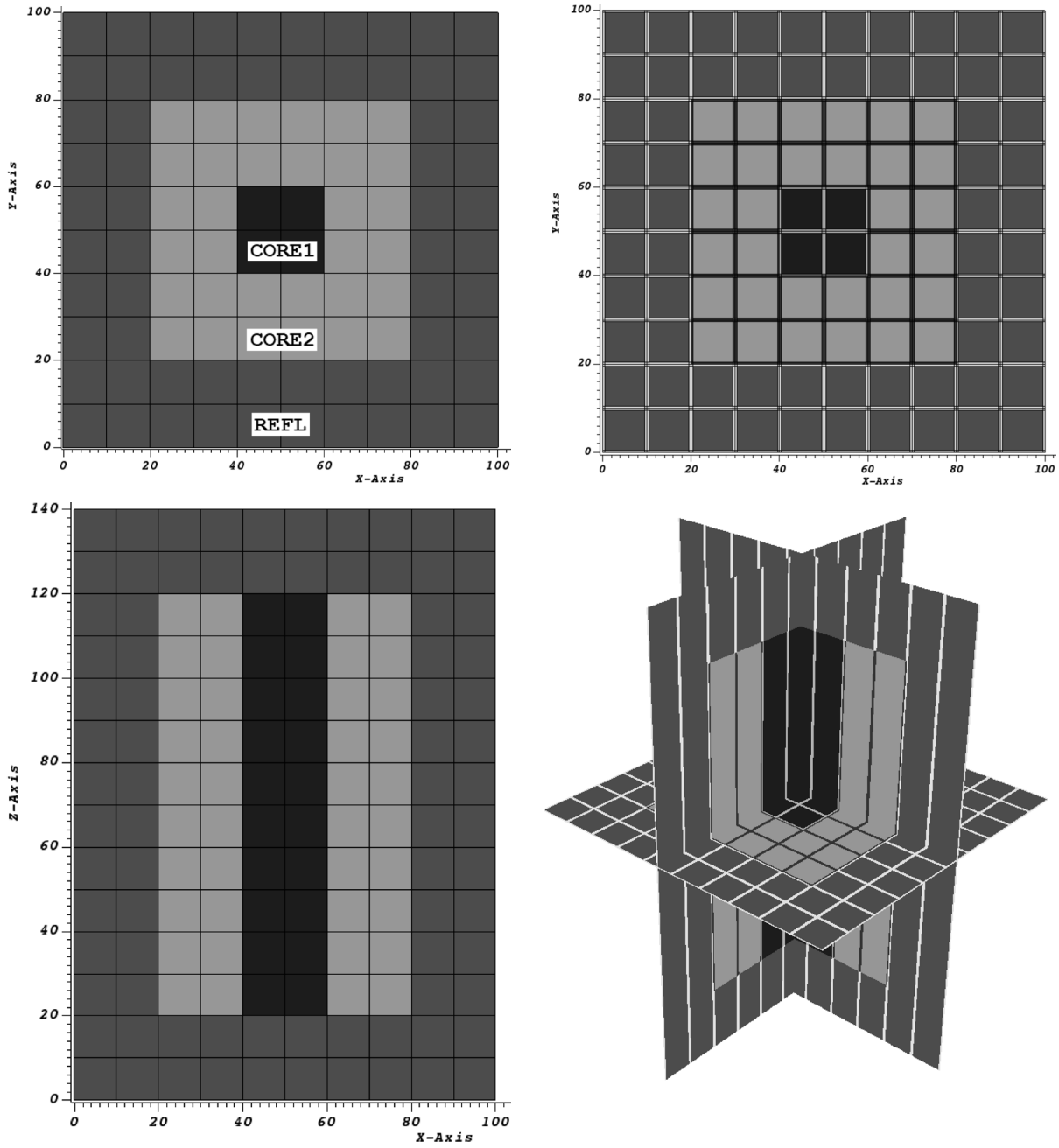

Figure 2-43. Bowing Worth Test Problem

The one group macroscopic cross section library data is provided in Table 2-25 for both the heterogeneous problem and the homogeneous one. For the heterogeneous problem there are six cross sections sets while the homogeneous one has three cross section sets. The first row of the heterogeneous cross section data section indicates that it is for the CORE1 duct regions (blue) in

the model. The second row indicates it is for the CORE1 bypass (cyan) that surrounds the CORE1 duct region. One can see that the duct and bypass cross section data is virtually identical with only a 5% decrease in the fission cross section and 5% increase in the capture cross section. No change in the total or scattering cross section is made. This same pattern occurs in the CORE2 duct and bypass regions where only the capture and fission cross sections are perturbed. For the REFL region, there is no fission and there is no difference in the cross section data between the duct and bypass. These changes are of course intentional to make the heterogeneous and homogeneous problem cross sections match. For the homogeneous problem that accompanies the heterogeneous one, the volume weighted cross section library is provided in Table 2-25 for comparison against the flux weighted one (using region-wise flux instead of mesh-wise flux). One can clearly see that they are effectively identical, which means that concerns on the accuracy with respect to cross section flux weighting should be minimal.

Table 2-25. Heterogeneous and Homogeneous One-Group Cross Sections

Region	Total	Capture	Fission	ν	Scatter
CORE1 Duct (blue)	0.5	0.01	0.01	3	0.48
CORE1 Bypass (cyan)	0.5	0.0105	0.0095	3	0.48
CORE2 Duct (green)	0.4	0.01	0.01	3	0.38
CORE2 Bypass (purple)	0.4	0.0107	0.0093	3	0.38
REFL Duct (red)	0.4	0.3			0.1
REFL Bypass (yellow)	0.4	0.3			0.1
Homogeneous Flux Weighted					
CORE1 (blue)	0.5	0.010084	0.009916	3	0.48
CORE2 (green)	0.4	0.010118	0.009882	3	0.38
REFL (red)	0.4	0.3			0.1
Homogeneous Volume Weighted					
CORE1 (blue)	0.5	0.010086	0.009914	3	0.48
CORE2 (green)	0.4	0.010120	0.009880	3	0.38
REFL (red)	0.4	0.3			0.1

With a by-pass gap of 0.45 cm on either side of the duct regions of the domain, one can perturb the duct position up to this amount before it becomes difficult to properly define a homogeneous geometry in DIF3D. To understand, if the duct crosses the original border, then the backfill of bypass material into the region the duct left, must include the bypass material from the adjacent mesh it entered as it is displacing the bypass material in that mesh. Because the bypass cross sections in this model are different in the three homogeneous regions, as opposed to a real-world problem where the cross sections would be very similar, this would cause significant errors in the PERSENT calculated results. Consequently, all of the perturbations considered were constrained to be less than a 0.45 cm movement of the central duct.

Figure 2-44 shows heterogeneous geometry configuration of the maximum perturbed state (pert5) studied in this work. Comparison with the heterogeneous geometry in Figure 2-43, one should be able to identify that the ducts in the range 20 cm < y < 50 cm are all shifted down while the ducts in the range 50 cm < y < 80 cm are all shifted up. No shift is made in the x direction of any duct. The y shift of the assemblies for pert5 was set as 0.40 cm which is just below the 0.45

cm maximum. Four additional perturbation problems were created which include a 0.05 cm (pert1), 0.15 cm (pert2), 0.25 cm (pert3), and 0.35 cm (pert4) movement of the ducts in the y range identical to that done for pert5.

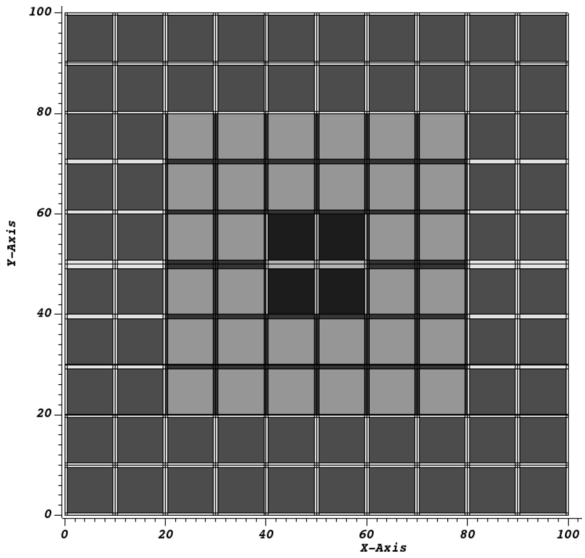

Figure 2-44. Bowing Worth Test Perturbed State Geometry (Pert5)

Both the homogeneous and heterogeneous DIF3D problems were built and the inputs for the heterogeneous ones can be found in the supplemental folder for benchmark 30 in the PERSENT distribution. Figure 2-45 provides a PERSENT output excerpt for the key parts of the output that are important to the verification process. The first section of output shows the mesh-wise bowing worth for pert1 on axial plane 8 (70-80 cm in the model). From the geometric perturbation, one would expect all assemblies in the range of 20 cm < y < 80 cm to be impacted by the perturbation because DIF3D is a structured grid code and the ducts in REFL are thus also shifted. However, because the REFL duct and bypass cross sections are identical, PERSENT correctly reports a zero worth derived from those meshes (columns 1, 2, 9, and 10 are all zeros).

```
…
[PERSENT]...Axial plane      8 data for First Order PT of PERT1
              1           2           3           4           5           6           7           8           9          10
    10  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     9  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     8  0.000E+00  0.000E+00 -1.535E-07 -7.035E-07 -1.215E-06 -1.215E-06 -7.035E-07 -1.535E-07  0.000E+00  0.000E+00
     7  0.000E+00  0.000E+00 -2.531E-07 -1.164E-06 -2.054E-06 -2.054E-06 -1.164E-06 -2.531E-07  0.000E+00  0.000E+00
     6  0.000E+00  0.000E+00 -1.236E-07 -5.935E-07 -9.258E-07 -9.258E-07 -5.935E-07 -1.236E-07  0.000E+00  0.000E+00
     5  0.000E+00  0.000E+00 -1.236E-07 -5.935E-07 -9.258E-07 -9.258E-07 -5.935E-07 -1.236E-07  0.000E+00  0.000E+00
     4  0.000E+00  0.000E+00 -2.531E-07 -1.164E-06 -2.054E-06 -2.054E-06 -1.164E-06 -2.531E-07  0.000E+00  0.000E+00
     3  0.000E+00  0.000E+00 -1.535E-07 -7.035E-07 -1.215E-06 -1.215E-06 -7.035E-07 -1.535E-07  0.000E+00  0.000E+00
     2  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
     1  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
…
[PERSENT]...Region edits for First Order PT of PERT1
[PERSENT]...|Region|Numerator | Numerator/=Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |          | Sum[Denom|          |          |          |             |             |             |
[PERSENT]...|REFL  | 0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|
[PERSENT]...|CORE2 |-2.249E+17|-1.331E-04|-1.786E-09|-5.312E-05| 5.312E-05|    0.000E+00|   0.000E+00|    1.331E-04|
[PERSENT]...|CORE1 |-3.321E+16|-1.965E-05|-2.107E-10|-7.842E-06| 7.842E-06|    0.000E+00|   0.000E+00|    1.965E-05|
=PERSENT...Parameter First Order PT of PERT1 is -1.52768E-04 denom 1.68973E+21 k-eff A 1.1971433E+00 F 1.1971433E+00
…
[PERSENT]...Region edits for First Order PT of PERT2
[PERSENT]...|Region|Numerator | Numerator/=Leakage  +  Capture + Fission  + Out Scatter - In Scatter - Production  |
[PERSENT]...|      |          | Sum[Denom|          |          |          |             |             |             |
[PERSENT]...|REFL  | 0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E+00|   0.000E+00|    0.000E+00|
[PERSENT]...|CORE2 |-6.741E+17|-3.989E-04|-5.351E-09|-1.592E-04| 1.592E-04|    0.000E+00|   0.000E+00|    3.989E-04|
[PERSENT]...|CORE1 |-1.005E+17|-5.949E-05|-6.378E-10|-2.374E-05| 2.374E-05|    0.000E+00|   0.000E+00|    5.949E-05|
=PERSENT...Parameter First Order PT of PERT2 is -4.58411E-04 denom 1.68973E+21 k-eff A 1.1971433E+00 F 1.1971433E+00
…
=PERSENT...Parameter First Order PT of PERT3 is -7.64172E-04 denom 1.68973E+21 k-eff A 1.1971433E+00 F 1.1971433E+00
=PERSENT...Parameter First Order PT of PERT4 is -1.07002E-03 denom 1.68973E+21 k-eff A 1.1971433E+00 F 1.1971433E+00
=PERSENT...Parameter First Order PT of PERT5 is -1.22297E-03 denom 1.68973E+21 k-eff A 1.1971433E+00 F 1.1971433E+00
```

Figure 2-45. PERSENT Bowing Worth Output Excerpt

The only non-zero values in Figure 2-45 occur on rows 3 through 8 which exactly correspond to 20 cm < y < 80 cm or y meshes 3, 4, 5, 6, 7, and 8.

The next section of output in Figure 2-45 covers the balance table for the pert1 test. The pert2 balance table is also provided and both were non-impactfully truncated to fit on the page. A quick review shows that the capture, fission, and production terms are the primary non-zero terms with leakage contributing next to nothing to the total worth. This is consistent with the cross section differences between the duct and bypass gap regions. The signs are also consistent with moving the higher worth duct material into the lower importance region and backfilling with the lower worth bypass gap material. The total worth for all five perturbation problems (pert1 through pert5) are also provided in Figure 2-45 for completeness.

To complete the verification, the comparison between the PERSENT first order worth calculation and the heterogeneous results needs to be compared which is done in Table 2-26. In all of these calculations, the maximum error was set 10^{-8} to ensure iterative convergence is not a contributing factor to any difference. To ensure that spatial mesh refinement issues were not a problem, a study was made using p-refinement in the heterogeneous and homogeneous problem where the appropriate regions in the heterogeneous problem were assigned the cross section data from the homogeneous. This effectively makes the heterogeneous geometry model just a mesh-refined case of the homogeneous model. Using an 8^{th} order flux, 8^{th} order source, and 3^{rd} order leakage, the heterogeneous model k_{eff} was 1.1971432 while the homogeneous one was 1.1971434. The difference is very small and it should be clear that spatial mesh and spatial flux/source order refinements should not be a contributing factor to any errors. It is noted that using the standard 6^{th} order flux, 6^{th} order source, and 1^{st} order leakage had a significantly larger error than that shown here, further supporting the idea that the higher order settings should eliminate this as a concern.

Table 2-26. Calculated Direct and PERSENT Bowing Worth Results

Problem	Heterogeneous DIF3D		PERSENT		
	k_{eff}	pcm	Worth	pcm	Error
Base	1.1969412				
Pert1	1.1967236	-15.2	-1.52768E-04	-15.3	-0.6%
Pert2	1.1962890	-45.5	-4.58411E-04	-45.8	-0.7%
Pert3	1.1958549	-75.9	-7.64172E-04	-76.4	-0.7%
Pert4	1.1954213	-106.2	-1.07002E-03	-107.0	-0.7%
Pert5	1.1952048	-121.4	-1.22297E-03	-122.3	-0.8%

The first heterogeneous k_{eff} result of 1.1969412 in Table 2-26 corresponds to the base state of the heterogeneous model which should match the homogeneous model result of 1.1971434. As can be seen, there is a ~20 pcm difference between the heterogeneous and homogeneous models. This mismatch in the models is small and should be a minor factor in any observed differences in the PERSENT bowing worth calculation. Looking at the direct calculated worth using the heterogeneous DIF3D k_{eff} results for the perturbations and comparing them to the PERSENT computed first order bowing worth ones, one finds them to effectively be identical for all five perturbation tests. The error in each case is below 1% which is more than acceptable for the verification work. The residual error in the PERSENT solutions should be due to the mismatch in the heterogeneous and homogeneous model which is likely a result of using region-wise homogenized cross section values instead of mesh-wise homogenized cross section values. Because this aspect is of little importance to the underlying verification work, no additional study was made to investigate it. With the provided detail in the PERSENT manual that compared the PERSENT bowing worth results for hexagonal geometries to MCNP continuous energy calculations and the results here, one can comfortably conclude that the bowing reactivity worth is working correctly. This work satisfies the d) task of the category 3 work in Table 1-1.

2.5 Kinetics Parameters Verification

The kinetics parameters are primarily used in a point kinetics based safety analysis methodology like that in SAS4A. The two primary components to compute are Λ, the prompt neutron lifetime, and β, the delayed neutron fraction. From the PERSENT manual, these are computed using:

$$\Lambda = \frac{1}{\lambda}\frac{\langle \psi^*, v^{-1} H\psi\rangle}{\langle \psi^*, F\psi\rangle} \qquad \& \qquad \beta = \frac{\sum_i^{isotopes} N_i \sum_m^{families,\,delay} \langle \psi^*, F_{i,m}\psi\rangle}{\langle \psi^*, F\psi\rangle} \tag{23}$$

For the prompt neutron lifetime, the denominator includes the eigenvalue and the total fission source from the base state. The numerator contains the *H* matrix which is stated to be an identity like matrix for PERSENT along with the inverse velocity. The velocity is obtained from the ISOTXS file for each energy group and represents the average velocity of the neutrons in each group. Because the expression for Λ involves higher order space-angle moments along with a sum over the whole domain (as opposed to just the fissionable regions), a hand calculation is not a trivial undertaking.

For the delayed neutron fraction, the total υ and χ provided on ISOTXS is split into prompt and delayed components where the delayed information is provided in DLAYXS. The DLAYXS data is an engineering fit of the decay behavior of several fission products that release neutrons well after the fission event occurred. Each isotope produces different quantities of the important fission products during fission and thus each isotope has its own set of decay constants as shown in Table 2-27 for five common isotopes of importance. Today, six delay families is standard while three delay families have been used and a thirteen delay family structure is also available.

Table 2-27. Delay Family Decay Constants (1/sec)

Family	U-233	U-235	U-238	Pu-239	Pu-240
1	0.0129	0.0133	0.0136	0.0133	0.0136
2	0.0347	0.0327	0.0313	0.0309	0.0300
3	0.119	0.121	0.123	0.113	0.117
4	0.286	0.303	0.324	0.293	0.307
5	0.788	0.849	0.906	0.857	0.870
6	2.44	2.85	3.05	2.73	3.00

The above decay constants are not impacted by the equation above as they simply specify the decay relationship for each family. For β, the $F_{i,m}$ operator in the numerator includes the delay υ and χ data from the DLAYXS file while the denominator contains the total υ and χ from ISOTXS generated by MC^2-3. Some example total and delay υ data for U-235 is provided in Figure 2-46 while Figure 2-47 provides the total and delay data for χ.

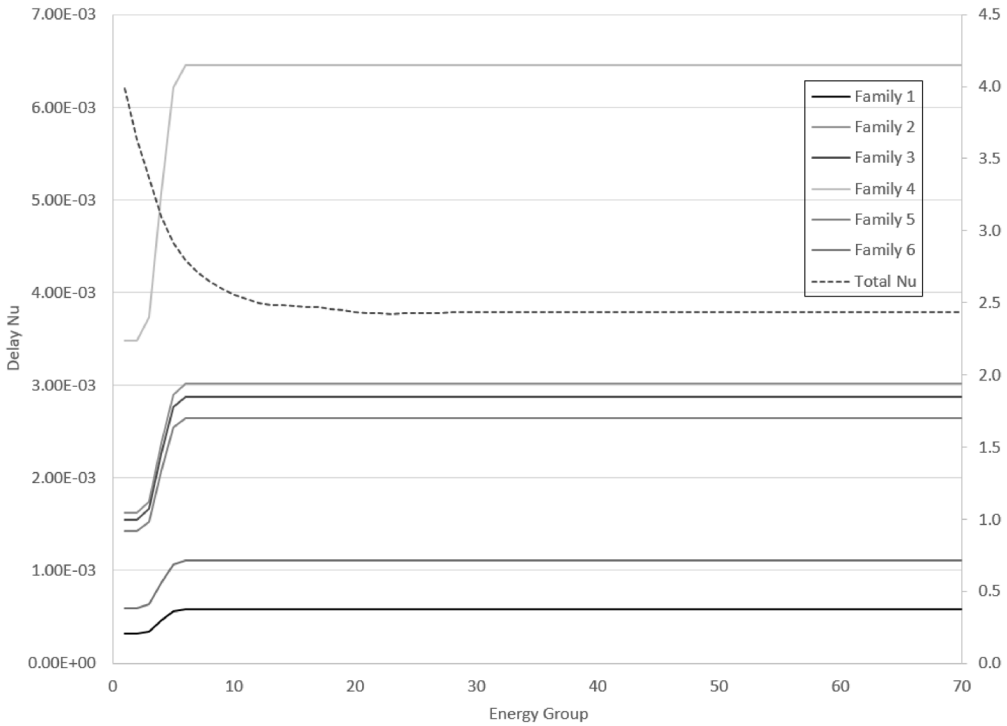

Figure 2-46. U-235 Delay and Total Nu Data

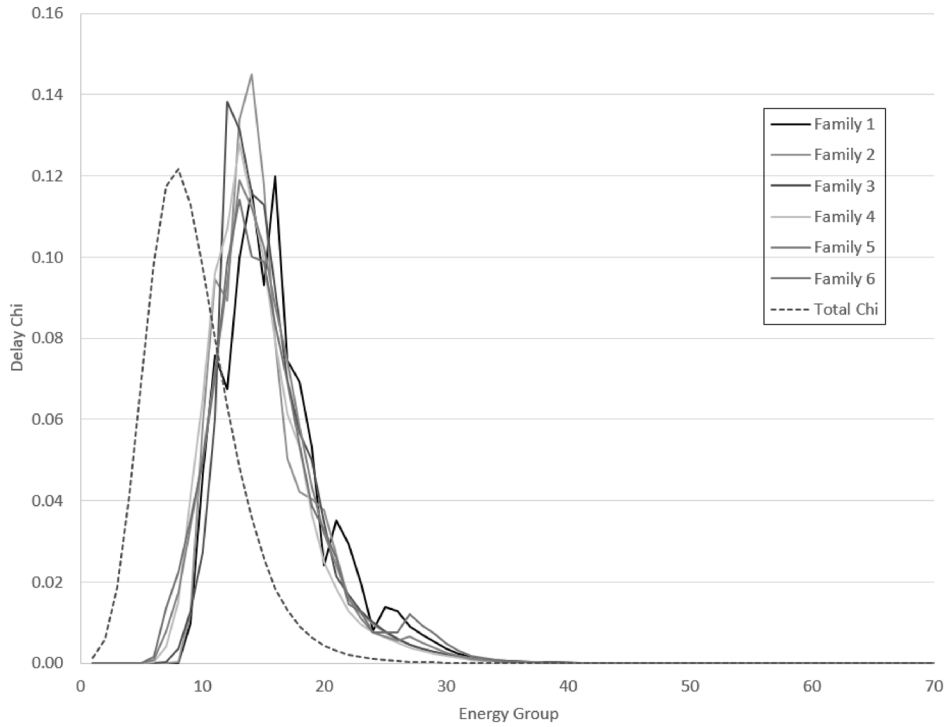

Figure 2-47. U-235 Delay and Total Chi Data

From the delay υ plot, it should be clear that at high energies (close to group 1), the fraction of neutrons emitted in delayed fission product decays goes down significantly. Over a bulk of the energy range, the magnitude of neutrons coming from any family is rather constant. For the delay χ, one can see from Figure 2-47 that the spectrum of released neutrons has an energy distribution considerably lower than that of the total χ. This is consistent with the fact that the isotopes that produce the delayed neutrons do not have as much free binding energy as the original U-235 isotope. Because the χ values for any family sum to unity, the real impact of the distribution is the weighting applied to the adjoint flux as outlined in equation 23 above. Unlike Λ, the β values can be manipulated rather easily to facilitate a hand calculation. First, they are only dependent upon those meshes with fissionable materials and second, since the delay data is not used in the regular solve process of DIF3D, components of it can be arbitrarily set to zero.

2.5.1 *Verification Using an Infinite Homogeneous Problem*

Because of the complexity of the Λ calculation, a reduction in the size of the domain is warranted to make a hand calculation more tractable. The same three group ISOTXS cross section data used in the first benchmark of Figure 2-1 is used here. This data set has cross sections for elemental sodium, iron, oxygen, carbon and actinide data for U-238, Pu-239, Pu-240, and Pu-241 along with a LFP and DUMP isotope typical in depletion calculations. The DLAYXS data set was also provided and only has data for Pu-239, U-238, and U-235.

The first test problem is a simple infinite homogeneous test case, the DIF3D and PERSENT input for which are provided in Figure 2-48. The PERSENT test case is benchmark 27 in the PERSENT distribution and the DIF3D model is benchmark 49 in the DIF3D distribution. As can be seen, a single zone C1 is used containing the Pu-239 and U-238 isotopes.

DIF3D A.NIP3 Input

```
03  120
04  4  4  4  4  4  4
05  XL 0.0
05  XU 0.0
05  YL 0.0
05  YU 0.0
05  ZL 0.0
05  ZU 0.0
09 Z  3  30.0

14  C1   PU239  0.0011   U238  0.0064
14  C1   NA     0.0104   FE    0.0181    O-16  0.0149
15    C1     CORE1
29  9.5
30  CORE1   1   0  0  0.0  30.0
30  CORE1   2   0  0  0.0  30.0
```

PERSENT Input

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   ./dif3d.x
DIF3D_INPUT        ./dif3d_a.inp

LAMBDA_BETA      YES
PROBLEM_EDITS    LAMBDA_BETA  PRINT_BY_REGION PRINT_BY_GROUP PRINT_BY_UNIQUE PRINT_BY_FAMILY
```

Figure 2-48. DIF3D and PERSENT Inputs for the Infinite Homogeneous Test Case

Figure 2-49 provides an excerpt of the PERSENT output for the Λ and β values. At the beginning of this output are warning messages indicating that several ISOTXS isotopes are not presently mapped to DLAYXS data (PU239H, U238H, PU240, PU241). Since the DLAYXS file does not have isotopes with these names, PERSENT is unable to match these fissionable isotopes with data in DLAYXS and warns the user. These warnings are immaterial to the problem being solved here as both PU239 and U238 are present and no user mapping input (set_delay) is present in Figure 2-48.

As was the case with other perturbation problems, the header for the kinetics parameters signifies the beginning of the kinetics parameter section. The Λ result is provided first followed by the β results. For Λ, a mesh-wise, region-wise and group-wise breakdown are possible but only the region and group detail was selected for this test case as seen in Figure 2-48 (no print_by_mesh setting). The prompt neutron lifetime from PERSENT is reported to be 5.53483E-07 seconds. The generation time is given as 4.29109E-07 which is simply the prompt neutron lifetime divided by k_{eff} (5.53483E-07/1.2898418=4.29109E-07). To calculate the prompt neutron lifetime, the forward and adjoint fluxes are needed along with the neutron velocities. The velocities from this ISOTXS file are 1.7399200E+09 cm/sec, 6.4163597E+08 cm/sec, 1.2828900E+08 cm/sec and the cross section data needed to compute the kinetics parameters are summarized in Table 2-28 and Table 2-29. The decay constants for all DLAYXS isotopes is 0.03 and 1.0, clearly indicating a contrived data set as opposed to that seen in Table 2-27.

The forward and adjoint flux solution from DIF3D is provided in Figure 2-50. Because the adjoint flux is not normalized in DIF3D, the adjoint cannot be obtained from the DIF3D verification test problem as DIF3D uses a different initialization of the adjoint when it solves the forward and adjoint problems in the same input deck. To demonstrate this, the adjoint solution from the DIF3D verification test output is provided at the bottom of Figure 2-50 and it is easy to see that the two adjoint flux solutions differ by a simple constant of ~1.28984 which should be recognized as the eigenvalue. Because the mesh-wise flux results will be identical everywhere in an infinite homogeneous problem, the region-wise detail is sufficient for the current needs. To compute the numerator of the prompt neutron lifetime, the forward and adjoint flux details, and the neutron velocities are combined as

$$\frac{\begin{pmatrix}2.19397E{+}14\\1.85873E{+}14\\1.47866E{+}14\end{pmatrix}^{T}\begin{pmatrix}\frac{1}{17.3992E{+}8} & 0 & 0\\ 0 & \frac{1}{6.4163597E{+}8} & 0\\ 0 & 0 & \frac{1}{1.28289E{+}8}\end{pmatrix}\begin{pmatrix}5.67797E{+}20\\1.95832E{+}21\\1.77517E{+}21\end{pmatrix}}{16413.3} = 1.6358E{+}23. \quad (24)$$

The denominator 16413.3 is the volume of the domain. This result closely matches the reported LAMBDA region numerator value of 1.636E+23 in Figure 2-49 highlighted in red.

```
…
[PERSENT]...Warning::: Fissionable ISOTXS isotope PU239H   is not mapped to any DLAYXS data
[PERSENT]...Warning::: Fissionable ISOTXS isotope U238H    is not mapped to any DLAYXS data
[PERSENT]...Warning::: Fissionable ISOTXS isotope PU240    is not mapped to any DLAYXS data
[PERSENT]...Warning::: Fissionable ISOTXS isotope PU241    is not mapped to any DLAYXS data
…
[PERSENT].....................................................................
[PERSENT]...Problem LAMBDA_BETA      is infamous
[PERSENT].....................................................................
[PERSENT]...Region edits for LAMBDA
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|CORE1 |    1|  4.362E+21|         1.144E-08|
[PERSENT]...|CORE1 |    2|  3.456E+22|         9.067E-08|
[PERSENT]...|CORE1 |    3|  1.247E+23|         3.270E-07|
[PERSENT]...|CORE1 |-----|  1.636E+23|         4.291E-07|
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  1.636E+23|         4.291E-07|
=PERSENT...Parameter LAMBDA Generation time  4.29109E-07 Prompt Lifetime  5.53483E-07 denom 3.81217E+29 k-eff  1.2898418E+00
[PERSENT]...Region edits for BETA PU239    family   1
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|CORE1 |    1|  2.348E+26|         6.160E-04|
[PERSENT]...|CORE1 |    2|  1.326E+26|         3.479E-04|
[PERSENT]...|CORE1 |    3|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |-----|  3.675E+26|         9.640E-04|
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  3.675E+26|         9.640E-04|
=PERSENT...BETA PU239    family   1  9.63990E-04 denominator  3.81217E+29 k-eff  1.2898418E+00
[PERSENT]...Region edits for BETA PU239    family   2
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|CORE1 |    1|  2.744E+26|         7.199E-04|
[PERSENT]...|CORE1 |    2|  5.813E+25|         1.525E-04|
[PERSENT]...|CORE1 |    3|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |-----|  3.326E+26|         8.724E-04|
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  3.326E+26|         8.724E-04|
=PERSENT...BETA PU239    family   2  8.72389E-04 denominator  3.81217E+29 k-eff  1.2898418E+00
[PERSENT]...Region edits for BETA cumulative PU239
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|CORE1 |    1|  5.093E+26|         1.336E-03|
[PERSENT]...|CORE1 |    2|  1.908E+26|         5.004E-04|
[PERSENT]...|CORE1 |    3|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |-----|  7.001E+26|         1.836E-03|
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  7.001E+26|         1.836E-03|
…
[PERSENT]...Region edits for Parameter BETA is
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|CORE1 |    1|  9.087E+26|         2.384E-03|
[PERSENT]...|CORE1 |    2|  3.127E+26|         8.202E-04|
[PERSENT]...|CORE1 |    3|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |-----|  1.221E+27|         3.204E-03|
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  1.221E+27|         3.204E-03|
=PERSENT...Parameter BETA is         3.20389E-03 denominator  3.81217E+29 k-eff  1.2898418E+00
=PERSENT...Domain coalesced kinetics parameters for unique isotope PU239S
=PERSENT...Family     beta(i)    lambda(i)
=PERSENT...   1   9.63990E-04  3.00000E-02
=PERSENT...   2   8.72389E-04  1.00000E+00
=PERSENT...Domain coalesced kinetics parameters for unique isotope U-238S
=PERSENT...Family     beta(i)    lambda(i)
=PERSENT...   1   4.33866E-04  3.00000E-02
=PERSENT...   2   9.33649E-04  1.00000E+00
=PERSENT...Domain coalesced effective point kinetics parameters
=PERSENT...Family     beta(i)    lambda(i)
=PERSENT...   1   1.39786E-03  3.00000E-02
=PERSENT...   2   1.80604E-03  1.00000E+00
```

Figure 2-49. PERSENT Output Excerpt for the Infinite Homogeneous Test Case

Table 2-28. ISOTXS Cross Section Data for the Fissionable Isotopes

	PU239			U238		
Group	χ	υ	σ_f	χ	υ	σ_f
1	0.78220	3.17907	1.83897	0.77530	2.75767	0.30062
2	0.20895	2.91926	1.55634	0.21553	2.47403	0.00034
3	0.00884	2.88136	2.32674	0.00915	2.41533	0.00011
	Pu240			Pu241		
	χ	υ	σ_f	χ	υ	σ_f
1	0.78120	3.11283	1.57974	0.78120	3.18041	1.59303
2	0.20994	2.87945	0.24066	0.20994	2.95671	1.81456
3	0.00889	2.80657	0.08990	0.00889	2.95306	4.26033
	PU239H			U238H		
	χ	υ	σ_f	χ	υ	σ_f
1	0.78220	3.17907	1.83896	0.77530	2.75766	0.30061
2	0.20895	2.91926	1.55634	0.21553	2.47401	0.00034
3	0.00884	2.88140	2.28678	0.00915	2.41534	0.00011

Table 2-29. DLAYXS Cross Section Data

Group	PU239			
	χ		υ	
	Fam. 1	Fam. 2	Fam. 1	Fam. 2
1	0.600	0.800	3.100E-03	2.700E-03
2	0.400	0.200	3.200E-03	2.800E-03
3	0.000	0.000	3.300E-03	2.900E-03
Group	U238			
	χ		υ	
	Fam. 1	Fam. 2	Fam. 1	Fam. 2
1	0.600	0.800	1.200E-02	2.500E-02
2	0.400	0.200	1.250E-02	2.750E-02
3	0.000	0.000	1.300E-02	3.000E-02
Group	U235			
	χ		υ	
	Fam. 1	Fam. 2	Fam. 1	Fam. 2
1	0.600	0.800	6.800E-03	8.800E-03
2	0.400	0.200	7.000E-03	9.000E-03
3	0.000	0.000	7.200E-03	9.200E-03

DIF3D Forward Flux Excerpt

```
0        REGION AND AREA REAL FLUX INTEGRALS FOR K-EFF  PROBLEM WITH ENERGY RANGE (EV)     =(4.140E-01,1.000E+07)
0
     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  CORE1     1  C1          1.64133E+04     4.30129E+21     2.62060E+17      2.33895E+21      1.42503E+17
         TOTALS                  1.64133E+04     4.30129E+21     2.62060E+17      2.33895E+21      1.42503E+17


     (1) PEAK FLUX CALCULATIONS ARE COMPUTED BY THE SPECIAL NODAL PROCEDURE  DOCUMENTED IN ANL 83-1
0
     REGION     ZONE  ZONE           GROUP           GROUP           GROUP
    NO.  NAME    NO.  NAME             1               2               3

      1  CORE1     1  C1          5.67797E+20     1.95832E+21     1.77517E+21
         TOTALS                  5.67797E+20     1.95832E+21     1.77517E+21
```

DIF3D Adjoint Flux Excerpt

```
0  REGION AND AREA   ADJOINT  FLUX INTEGRALS FOR K-EFF  PROBLEM WITH ENERGY RANGE (EV)     =(4.140E-01,1.000E+07)
0
     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  CORE1     1  C1          1.64133E+04     5.53137E+14     3.37004E+10      3.87505E+14      2.36091E+10
         TOTALS                  1.64133E+04     5.53137E+14     3.37004E+10      3.87505E+14      2.36091E+10


     (1) PEAK FLUX CALCULATIONS ARE COMPUTED BY THE SPECIAL NODAL PROCEDURE  DOCUMENTED IN ANL 83-1
0
     REGION     ZONE  ZONE           GROUP           GROUP           GROUP
    NO.  NAME    NO.  NAME             1               2               3

      1  CORE1     1  C1          2.19397E+14     1.85873E+14     1.47866E+14
         TOTALS                  2.19397E+14     1.85873E+14     1.47866E+14
```

DIF3D Verification Test Problem Adjoint Flux Excerpt

```
0  REGION AND AREA   ADJOINT  FLUX INTEGRALS FOR K-EFF  PROBLEM WITH ENERGY RANGE (EV)     =(4.140E-01,1.000E+07)
0
     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  CORE1     1  C1          1.64133E+04     4.28841E+14     2.61276E+10      3.00428E+14      1.83039E+10
         TOTALS                  1.64133E+04     4.28841E+14     2.61276E+10      3.00428E+14      1.83039E+10


     (1) PEAK FLUX CALCULATIONS ARE COMPUTED BY THE SPECIAL NODAL PROCEDURE  DOCUMENTED IN ANL 83-1
0
     REGION     ZONE  ZONE           GROUP           GROUP           GROUP
    NO.  NAME    NO.  NAME             1               2               3

      1  CORE1     1  C1          1.70096E+14     1.44105E+14     1.14639E+14
         TOTALS                  1.70096E+14     1.44105E+14     1.14639E+14
```

Figure 2-50. DIF3D Output Excerpt for the Infinite Homogeneous Test Case

The first group-wise component can be calculated as

$$\frac{2.19397\text{E+}14\cdot\frac{1}{17.3992\text{E+}8}\cdot 5.67797\text{E+}20}{16413.3} = 4.3621\text{E+}21. \quad (25)$$

This result closely matches the LAMBDA group numerator value also highlighted in red in Figure 2-49. The remaining group-wise values from PERSENT can be obtained in a similar manner to that done here showing that the hand calculated results are consistent with the PERSENT output.

The denominator of Λ can be computed as

$$W_{PU239} = 0.0011 \cdot \begin{pmatrix} 3.179070 \\ 2.919260 \\ 2.88136 \end{pmatrix}^T \begin{pmatrix} 1.83897 \\ 1.55634 \\ 2.32674 \end{pmatrix} = 0.01880313$$

$$W_{U238} = 0.0064 \cdot \begin{pmatrix} 2.75767 \\ 2.47403 \\ 2.41533 \end{pmatrix}^T \begin{pmatrix} 0.3006180 \\ 3.393970\text{E-}4 \\ 1.145080\text{E-}4 \end{pmatrix} = 0.00531278$$

$$\bar{\chi} = \begin{pmatrix} 0.7821960 \\ 0.2089490 \\ 0.0088392 \end{pmatrix} \cdot \frac{W_{PU239}}{W_{PU239} + W_{U238}} + \begin{pmatrix} 0.775302 \\ 0.21553 \\ 0.00915239 \end{pmatrix} \cdot \frac{W_{U238}}{W_{PU239} + W_{U238}} = \begin{pmatrix} 0.780677 \\ 0.210399 \\ 0.0089082 \end{pmatrix}$$

$$\bar{\Sigma}_P = 0.0011 \cdot \begin{pmatrix} 3.179070 \cdot 1.83897 \\ 2.919260 \cdot 1.55634 \\ 2.88136 \cdot 2.32674 \end{pmatrix} + 0.0064 \cdot \begin{pmatrix} 2.75767 \cdot 0.3006180 \\ 2.47403 \cdot 3.393970\text{E-}4 \\ 2.41533 \cdot 1.145080\text{E-}4 \end{pmatrix} = \begin{pmatrix} 0.0117365 \\ 0.0050031 \\ 0.0073764 \end{pmatrix}$$

$$\frac{\psi^{*T} \cdot V \bar{\chi} \bar{\Sigma}_P^T \psi \cdot V}{V} = \frac{\begin{pmatrix} 2.19397\text{E+}14 \\ 1.85873\text{E+}14 \\ 1.47866\text{E+}14 \end{pmatrix}^T \begin{pmatrix} 0.780677 \\ 0.210399 \\ 0.0089082 \end{pmatrix} \begin{pmatrix} 0.0117365 \\ 0.0050031 \\ 0.0073764 \end{pmatrix}^T \begin{pmatrix} 5.67797\text{E+}20 \\ 1.95832\text{E+}21 \\ 1.77517\text{E+}21 \end{pmatrix}}{16413.3} = 3.81219\text{E+}29. \quad (26)$$

From Figure 2-49, this hand calculated results closely matches the reported value of 3.81217E+29 from PERSENT. The slight error is attributable to the round off error from the DIF3D reported outputs for volume and flux. In the equations above, the compositional $\bar{\chi}$ approach used in DIF3D is displayed along with the macroscopic production cross section Σ_P. The 0.0011 and 0.0064 are the atom density for each isotope in the mixture. For the numerator of β in equation 23, the compositional $\bar{\chi}$ is not needed. This is primarily a consequence of the way in which one chooses to define the prompt neutron source in the spatial kinetics equations which is beyond the scope of the present point kinetics formalism.

The numerator of β has an individual value for each family of each isotope (Pu239 and U238) followed by a cumulative value for each isotope. The same table data repeats for each fissionable isotope in the model. Only the two tables for the family and cumulative β for Pu239 are displayed in Figure 2-49. The two family β values of the numerator are highlighted in green while the cumulative one is highlighted in orange. To calculate each one, the delay data is combined with the fluxes in the following manner, similar to that done above with the denominator.

$$\beta_{PU239,1} = \frac{0.0011 \cdot \frac{\begin{pmatrix} 2.19397\text{E+}14 \\ 1.85873\text{E+}14 \\ 1.47866\text{E+}14 \end{pmatrix}^T \begin{pmatrix} 0.6 \\ 0.4 \\ 0.0 \end{pmatrix} \begin{pmatrix} 3.10\text{E-}03 \cdot 1.83897 \\ 3.20\text{E-}03 \cdot 1.55634 \\ 3.30\text{E-}03 \cdot 2.32674 \end{pmatrix}^T \begin{pmatrix} 5.67797\text{E+}20 \\ 1.95832\text{E+}21 \\ 1.77517\text{E+}21 \end{pmatrix}}{16413.3}}{3.81219\text{E+}29}. \quad (27)$$

$$= \frac{3.674911\text{E+}26}{3.81219\text{E+}29} = 9.6399\text{E-}04$$

This hand calculation is also consistent with the reported numerator value of 3.675E+26 in Figure 2-49 and the β value of 9.63990E-4 reported family 1 of the PU239 isotope.

The second family of Pu239 is calculated using

$$\beta_{PU239,2} = \frac{0.0011 \cdot \frac{\begin{pmatrix} 2.19397\text{E+}14 \\ 1.85873\text{E+}14 \\ 1.47866\text{E+}14 \end{pmatrix}^T \begin{pmatrix} 0.8 \\ 0.2 \\ 0.0 \end{pmatrix} \begin{pmatrix} 2.70\text{E-}03 \cdot 1.83897 \\ 2.80\text{E-}03 \cdot 1.55634 \\ 2.90\text{E-}03 \cdot 2.32674 \end{pmatrix}^T \begin{pmatrix} 5.67797\text{E+}20 \\ 1.95832\text{E+}21 \\ 1.77517\text{E+}21 \end{pmatrix}}{16413.3}}{3.81219\text{E+}29}. \quad (28)$$

$$= \frac{3.32571\text{E+}26}{3.81219\text{E+}29} = 8.72389\text{E-}04$$

This result is also consistent with the PERSENT values of 3.326E26 and 8.72389E-4 for family 2 of PU239.

The cumulative result is simply the sum of the family wise data and can be calculated as

$$3.674911\text{E+}26 + 3.32571\text{E+}26 = 7.00062\text{E+}26$$
$$9.6399\text{E-}4 + 8.72389\text{E-}4 = 1.83638\text{E-}3. \quad (29)$$

These values are consistent with the PERSENT cumulative PU239 numerator value 7.001E+26 and β value of 1.836E-03 in Figure 2-49.

The U238 family wise values are calculated in a similar manner as

$$\beta_{U238,1} = \frac{0.0064 \cdot \begin{pmatrix} 2.19397\text{E+}14 \\ 1.85873\text{E+}14 \\ 1.47866\text{E+}14 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} 0.6 \\ 0.4 \\ 0.0 \end{pmatrix} \begin{pmatrix} 0.012 \cdot 0.300618 \\ 0.0125 \cdot 3.39397\text{E-}4 \\ 0.013 \cdot 1.14508\text{E-}4 \end{pmatrix}^{T} \begin{pmatrix} 5.67797\text{E+}20 \\ 1.95832\text{E+}21 \\ 1.77517\text{E+}21 \end{pmatrix}}{16413.3}}{3.81219\text{E+}29}. \quad (30)$$
$$= \frac{1.65398\text{E+}26}{3.81219\text{E+}29} = 4.3387\text{E-}04$$

$$\beta_{U238,2} = \frac{0.0064 \cdot \begin{pmatrix} 2.19397\text{E+}14 \\ 1.85873\text{E+}14 \\ 1.47866\text{E+}14 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} 0.8 \\ 0.2 \\ 0.0 \end{pmatrix} \begin{pmatrix} 0.025 \cdot 0.300618 \\ 0.0275 \cdot 3.39397\text{E-}4 \\ 0.030 \cdot 1.14508\text{E-}4 \end{pmatrix}^{T} \begin{pmatrix} 5.67797\text{E+}20 \\ 1.95832\text{E+}21 \\ 1.77517\text{E+}21 \end{pmatrix}}{16413.3}}{3.81219\text{E+}29}. \quad (31)$$
$$= \frac{3.35592\text{E+}26}{3.81219\text{E+}29} = 9.33648\text{E-}04$$

Comparison with the values reported by PERSENT (not shown for brevity) also shows that the numerator and β value for each family of U238 is consistent with the PERSENT output. After the family breakdown of each isotope is provided in the PERSENT output, the total β breakdown by region is provided which is displayed at the end of Figure 2-49. This is a sum over all families and isotopes which can be computed as the sum of equations 27 to 31 as 3.204E-03 which is consistent with the PERSENT reported value of 3.20389E-03 in Figure 2-49. From all of the preceding work, it should be clear that how PERSENT states it is calculating the kinetics parameters is consistent with the hand calculation of those parameters for this simple test case.

The coalesced parameters that appear at the end of the PERSENT output in Figure 2-49 will match the total values from the family breakdown of each isotope. This is primarily because the problem consists of a single region. If more regions were defined, and the user defined an area that consists of all of the fissionable regions, then that area edit in the family breakdown of each isotope will reproduce the coalesced values at the end of the output. It is a simple matter to verify that the coalesced family breakdown of each isotope matches the hand calculations of equations 28 to 31.

To calculate the β effective details, the PERSENT manual states it is using the following two equations which are consistent with the literature.

$$\bar{\beta}_m = \sum_i \beta_{i,m}. \quad (32)$$
$$C_m(0) = \frac{\bar{\beta}_m}{\Lambda_G \bar{\lambda}_m} p(0) = \sum_i \frac{\beta_{i,m}}{\Lambda_G \lambda_{i,m}} p(0) = \frac{p(0)}{\Lambda_G} \sum_i \frac{\beta_{i,m}}{\lambda_{i,m}} \rightarrow \bar{\lambda}_m = \frac{\bar{\beta}_m}{\sum_i \beta_{i,m}/\lambda_{i,m}}. \quad (33)$$

The β_m values are calculated simply as

$$\beta_1 = \beta_{PU239,1} + \beta_{U238,1} = 9.6399\text{E-}04 + 4.3387\text{E-}04 = 1.39786\text{E-}03$$
$$\beta_2 = \beta_{PU239,2} + \beta_{U238,2} = 8.72389\text{E-}04 + 9.33648\text{E-}04 = 1.80604\text{E-}03. \quad (34)$$

These match the PERSENT reported values of 1.39786E-03 and 1.80604E-03 in Figure 2-49. The effective decay constants are then calculated as

$$\lambda_1 = \frac{\beta_{PU239,1} + \beta_{U238,1}}{\frac{\beta_{PU239,1}}{\lambda_{PU239,1}} + \frac{\beta_{U238,1}}{\lambda_{U238,1}}} = \frac{9.6399\text{E-}04+4.3387\text{E-}04}{\frac{9.6399\text{E-}04}{0.03} + \frac{4.3387\text{E-}04}{0.03}} = 0.03$$

$$\lambda_2 = \frac{\beta_{PU239,2}+\beta_{U238,2}}{\frac{\beta_{PU239,2}}{\lambda_{PU239,2}}+\frac{\beta_{U238,2}}{\lambda_{U238,2}}} = \frac{8.72389\text{E-}04+9.33648\text{E-}04}{\frac{8.72389\text{E-}04}{1.0}+\frac{9.33648\text{E-}04}{1.0}} = 1.0. \quad (35)$$

These values also match the PERSENT reported values of 3.0E-03 and 1.0 in in Figure 2-49. It is important to note that because the DLAYXS data specified all isotopes with the same decay constants, that the decay constant calculation in equation 35 is not very meaningful.

2.5.2 *Verification Using a Two Region Slab Lattice Test*

To extend the previous hand calculation, a two region, two zone slab lattice calculation is used as the next verification test. The DIF3D and PERSENT input is provided in Figure 2-51 and one can see that the only spatial difference is in the axial direction. The second composition contains PU240 and PU241 which are seen to be mapped to the U235 precursor data in DLAYXS in the PERSENT input.

In this example, only the flat flux outputs from DIF3D will be used to compute the numerator of the kinetics parameters. The same technique used previously of modifying the NHFLUX files to only contain the flat moments is used to ensure the PERSENT calculated results match the hand calculation. Only the numerator details are checked as there is sufficient example work in the preceding perturbation theory sections to ensure that the denominator calculated by PERSENT is correct. The PERSENT output excerpt for this problem is shown in Figure 2-52 which includes both the PERSENT output when using the modified NHFLUX file, termed “flat flux” and the regular PERSENT output. Note that PRINT_BY_GROUP was not used but PRINT_BY_AREA was and thus the area edits will be checked in this section.

DIF3D A.NIP3 Input

```
03  120
04  4  4  4  4  4  4
05  XL 0.0
05  XU 0.0
05  YL 0.0
05  YU 0.0
05  ZL 0.0
05  ZU 0.0
07  CORE1 CORE1A CORE1B CORE1C
07  CORE2 CORE2A CORE2B CORE2C
07  TCORE CORE1A CORE1B CORE1C CORE2A CORE2B CORE2C
09 Z  6  60.0
14  C1   PU239  0.0010   U238  0.0050
                              14  C2   PU241  0.0020   PU240 0.0060
15    C1 CORE1A CORE1B CORE1C
15    C2 CORE2A CORE2B CORE2C
29  9.5
30  CORE1A   1   0  0   0.0  10.0
30  CORE1A   2   0  0   0.0  10.0
30  CORE1B   1   0  0  10.0  20.0
30  CORE1B   2   0  0  10.0  20.0
30  CORE1C   1   0  0  20.0  30.0
30  CORE1C   2   0  0  20.0  30.0
30  CORE2A   1   0  0  30.0  40.0
30  CORE2A   2   0  0  30.0  40.0
30  CORE2B   1   0  0  40.0  50.0
30  CORE2B   2   0  0  40.0  50.0
30  CORE2C   1   0  0  50.0  60.0
30  CORE2C   2   0  0  50.0  60.0
```

PERSENT Input

```
FORCE_FULL_FLUX    YES
DIF3D_EXECUTABLE   ./dif3d.x
DIF3D_INPUT        ./dif3d_b.inp


LAMBDA_BETA      YES
PROBLEM_EDITS    LAMBDA_BETA  PRINT_BY_REGION PRINT_BY_UNIQUE PRINT_BY_FAMILY
SET_DELAY PU240 U235
SET_DELAY PU241 U235
```

Figure 2-51. DIF3D and PERSENT Input for the Two Region Slab Lattice Test

PERSENT Result

```
[PERSENT]...Region edits for LAMBDA
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  1.019E+22|         1.340E-08|
[PERSENT]...|CORE1B|  1.019E+22|         1.340E-08|
[PERSENT]...|CORE1C|  1.015E+22|         1.335E-08|
[PERSENT]...|CORE2A|  1.003E+22|         1.319E-08|
[PERSENT]...|CORE2B|  9.981E+21|         1.313E-08|
[PERSENT]...|CORE2C|  9.988E+21|         1.314E-08|
[PERSENT]...Area edits for LAMBDA
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  3.052E+22|         4.014E-08|
[PERSENT]...|CORE2 |  3.000E+22|         3.945E-08|
[PERSENT]...|TCORE |  6.052E+22|         7.960E-08|
=PERSENT...Parameter LAMBDA Generation time  7.95963E-08 Prompt Lifetime  1.86903E-07 denom 7.60393E+29 k-eff  2.3481355E+00
```

PERSENT Modified NHFLUX Flat Flux Result

```
[PERSENT]...Region edits for LAMBDA
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  1.019E+22|         1.340E-08|
[PERSENT]...|CORE1B|  1.019E+22|         1.340E-08|
[PERSENT]...|CORE1C|  1.015E+22|         1.335E-08|
[PERSENT]...|CORE2A|  1.003E+22|         1.320E-08|
[PERSENT]...|CORE2B|  9.982E+21|         1.313E-08|
[PERSENT]...|CORE2C|  9.989E+21|         1.314E-08|
[PERSENT]...Area edits for LAMBDA
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  3.053E+22|         4.015E-08|
[PERSENT]...|CORE2 |  3.000E+22|         3.946E-08|
[PERSENT]...|TCORE |  6.053E+22|         7.961E-08|
=PERSENT...Parameter LAMBDA Generation time  7.95963E-08 Prompt Lifetime  1.86903E-07 denom 7.60393E+29 k-eff  2.3481355E+00
```

Figure 2-52. PERSENT Prompt Neutron Lifetime Excerpt for the Two Region Slab Lattice Test

The DIF3D output excerpts of the flux details are omitted for brevity and the parts of the flux vector will be provided with the hand calculation results to follow. The volume of every region is ~5471.12 cm^3. The hand calculation of the prompt neutron lifetime of each region is provided in Table 2-30 the details of which can be found in an EXCEL document in the supplemental folder for this PERSENT test problem. Both numerator values from the two PERSENT calculations are provided. As can be seen, the hand calculated results not only match the Flat Flux PERSENT result, but are very similar to the results when not using that approach. This is purely an artifact of the simplicity of this problem and one should note that the hand calculation can only match the Flat Flux PERSENT calculation.

Table 2-30. Hand Calculation of the Λ Numerator in the Two Region Slab Lattice Test

	Integrated Adjoint Flux	Velocity	Integrated Forward Flux	Group-wise Contribution	Numerator	PERSENT	PERSENT Flat Flux
CORE1A	1.285E+14	1.740E+09	9.698E+19	1.310E+21	1.019E+22	1.019E+22	1.019E+22
	1.006E+14	6.416E+08	2.139E+20	6.126E+21			
	6.113E+13	1.283E+08	3.159E+19	2.751E+21			
CORE1B	1.300E+14	1.740E+09	1.001E+20	1.368E+21	1.019E+22	1.019E+22	1.019E+22
	1.013E+14	6.416E+08	2.117E+20	6.110E+21			
	6.258E+13	1.283E+08	3.038E+19	2.709E+21			
CORE1C	1.329E+14	1.740E+09	1.067E+20	1.491E+21	1.015E+22	1.015E+22	1.015E+22
	1.028E+14	6.416E+08	2.070E+20	6.060E+21			
	6.562E+13	1.283E+08	2.782E+19	2.601E+21			
CORE2A	1.376E+14	1.740E+09	1.173E+20	1.696E+21	1.003E+22	1.003E+22	1.003E+22
	1.050E+14	6.416E+08	1.992E+20	5.960E+21			
	7.069E+13	1.283E+08	2.362E+19	2.379E+21			
CORE2B	1.416E+14	1.740E+09	1.258E+20	1.870E+21	9.982E+21	9.981E+21	9.982E+21
	1.071E+14	6.416E+08	1.936E+20	5.906E+21			
	7.457E+13	1.283E+08	2.076E+19	2.206E+21			
CORE2C	1.435E+14	1.740E+09	1.297E+20	1.956E+21	9.989E+21	9.988E+21	9.989E+21
	1.081E+14	6.416E+08	1.914E+20	5.894E+21			
	7.626E+13	1.283E+08	1.968E+19	2.138E+21			

Looking at the area results, the CORE1, CORE2, and TCORE area edits are computed as simple sums of the results calculated in Table 2-30 as

$$Numerator_{CORE1} = 1.019E+22+1.019E+22+1.015E+22 = 3.053E+22$$
$$Numerator_{CORE2} = 1.003E+22+9.982E+21+9.989E+21 = 3.000E+22$$
$$Numerator_{TCORE} = Numerator_{CORE1} + Numerator_{CORE2} = 6.053E+22. \quad (36)$$

These area numerator results are identical to the Flat Flux PERSENT reported values and similar to the PERSENT results without the NHFLUX modification. The hand calculation again confirms that PERSENT is computing the prompt neutron lifetime numerator values as stated in the manual.

The numerator values of β are again the focus of the verification work for this section. Figure 2-53 provides the PERSENT output excerpt for the PU239 β results. Both PERSENT results are again included. A quick inspection shows that they are very similar except for the denominator values and any quantity that involves it.

PERSENT Result

```
[PERSENT]...Region edits for BETA PU239    family   1
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  3.990E+25|         5.248E-05|
[PERSENT]...|CORE1B|  4.026E+25|         5.295E-05|
[PERSENT]...|CORE1C|  4.094E+25|         5.384E-05|
[PERSENT]...|CORE2A|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2B|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2C|  0.000E+00|         0.000E+00|
[PERSENT]...Area edits for BETA PU239    family   1
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  1.211E+26|         1.593E-04|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00|
[PERSENT]...|TCORE |  1.211E+26|         1.593E-04|
=PERSENT...BETA PU239    family   1  1.59267E-04 denominator  7.60393E+29 k-eff  2.3481355E+00
[PERSENT]...Region edits for BETA PU239    family   2
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  3.655E+25|         4.807E-05|
[PERSENT]...|CORE1B|  3.690E+25|         4.853E-05|
[PERSENT]...|CORE1C|  3.757E+25|         4.941E-05|
[PERSENT]...|CORE2A|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2B|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2C|  0.000E+00|         0.000E+00|
[PERSENT]...Area edits for BETA PU239    family   2
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  1.110E+26|         1.460E-04|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00|
[PERSENT]...|TCORE |  1.110E+26|         1.460E-04|
=PERSENT...BETA PU239    family   2  1.46010E-04 denominator  7.60393E+29 k-eff  2.3481355E+00
```

PERSENT Modified NHFLUX Flat Flux Result

```
[PERSENT]...Region edits for BETA PU239    family   1
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  3.990E+25|         5.248E-05|
[PERSENT]...|CORE1B|  4.026E+25|         5.295E-05|
[PERSENT]...|CORE1C|  4.094E+25|         5.384E-05|
[PERSENT]...|CORE2A|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2B|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2C|  0.000E+00|         0.000E+00|
[PERSENT]...Area edits for BETA PU239    family   1
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  1.211E+26|         1.593E-04|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00|
[PERSENT]...|TCORE |  1.211E+26|         1.593E-04|
=PERSENT...BETA PU239    family   1  1.59272E-04 denominator  7.60370E+29 k-eff  2.3481355E+00
[PERSENT]...Region edits for BETA PU239    family   2
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  3.655E+25|         4.807E-05|
[PERSENT]...|CORE1B|  3.690E+25|         4.853E-05|
[PERSENT]...|CORE1C|  3.757E+25|         4.941E-05|
[PERSENT]...|CORE2A|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2B|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2C|  0.000E+00|         0.000E+00|
[PERSENT]...Area edits for BETA PU239    family   2
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  1.110E+26|         1.460E-04|
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00|
[PERSENT]...|TCORE |  1.110E+26|         1.460E-04|
=PERSENT...BETA PU239    family   2  1.46015E-04 denominator  7.60370E+29 k-eff  2.3481355E+00
```

Figure 2-53. PERSENT Excerpt of β for PU239 for the Two Region Slab Lattice Test

Table 2-31 provides the hand calculation of β. In Table 2-31, the PERSENT results for the Flat Flux are omitted as they were identical to the output from PERSENT without the modified NHFLUX files. This is again an artifact of the simplicity of this problem and the output limits of PERSENT noting that the two PERSENT results do differ in the 5th (or 6th) significant digit on most of the reported denominator and β values.

Table 2-31. Hand Calculation of the PU239 β Numerator in the Two Region Slab Lattice Test

	Integrated Adjoint Flux	Delay χ	Delay υ	Fission	Integrated Forward Flux	Numerator	PERSENT
Family 1							
CORE1A	1.285E+14	0.60	0.0031	1.83897	9.698E+19	3.990E+25	3.990E+25
	1.006E+14	0.40	0.0032	1.55634	2.139E+20		
	6.113E+13	0.00	0.0033	2.32674	3.159E+19		
CORE1B	1.300E+14	0.60	0.0031	1.83897	1.001E+20	4.026E+25	4.026E+25
	1.013E+14	0.40	0.0032	1.55634	2.117E+20		
	6.258E+13	0.00	0.0033	2.32674	3.038E+19		
CORE1C	1.329E+14	0.60	0.0031	1.83897	1.067E+20	4.094E+25	4.094E+25
	1.028E+14	0.40	0.0032	1.55634	2.070E+20		
	6.562E+13	0.00	0.0033	2.32674	2.782E+19		
Family 2							
CORE1A	1.285E+14	0.80	0.0027	1.83897	9.698E+19	3.655E+25	3.655E+25
	1.006E+14	0.20	0.0028	1.55634	2.139E+20		
	6.113E+13	0.00	0.0029	2.32674	3.159E+19		
CORE1B	1.300E+14	0.80	0.0027	1.83897	1.001E+20	3.690E+25	3.690E+25
	1.013E+14	0.20	0.0028	1.55634	2.117E+20		
	6.258E+13	0.00	0.0029	2.32674	3.038E+19		
CORE1C	1.329E+14	0.80	0.0027	1.83897	1.067E+20	3.757E+25	3.757E+25
	1.028E+14	0.20	0.0028	1.55634	2.070E+20		
	6.562E+13	0.00	0.0029	2.32674	2.782E+19		

The excerpt of the PERSENT output for the PU241 β result is provided in Figure 2-54 where the Flat Flux PERSENT result are omitted for brevity. The hand calculation has the same setup as that of the PU239 β above and is provided in Table 2-32. Because PU241 is in a different spatial region than PU239, the forward and adjoint fluxes are different. One can compare the data in both tables to that of Table 2-28 and Table 2-29. As stated, the U235 delay data was mapped into PU241 and the resulting numerator results from the hand calculation again match the PERSENT reported results to the specified precision in the PERSENT output. The modified NHFLUX file PERSENT calculation yielded numerator results that were identical to those within the output precision in PERSENT. It should be clear that the hand calculation is only consistent with the Flat Flux PERSENT calculation.

```
[PERSENT]...Region edits for BETA PU241    family   1
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1B|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1C|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2A|  2.061E+26|         2.710E-04|
[PERSENT]...|CORE2B|  2.082E+26|         2.739E-04|
[PERSENT]...|CORE2C|  2.100E+26|         2.761E-04|
[PERSENT]...Area edits for BETA PU241    family   1
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |  6.243E+26|         8.210E-04|
[PERSENT]...|TCORE |  6.243E+26|         8.210E-04|
=PERSENT...BETA PU241    family   1  8.20977E-04 denominator  7.60393E+29 k-eff  2.3481355E+00
[PERSENT]...Region edits for BETA PU241    family   2
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1A|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1B|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1C|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2A|  2.790E+26|         3.669E-04|
[PERSENT]...|CORE2B|  2.825E+26|         3.715E-04|
[PERSENT]...|CORE2C|  2.851E+26|         3.749E-04|
[PERSENT]...Area edits for BETA PU241    family   2
[PERSENT]...| Area | Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |  8.466E+26|         1.113E-03|
[PERSENT]...|TCORE |  8.466E+26|         1.113E-03|
=PERSENT...BETA PU241    family   2  1.11340E-03 denominator  7.60393E+29 k-eff  2.3481355E+00
```

Figure 2-54. PERSENT Excerpt of β for PU241 for the Two Region Slab Lattice Test

Table 2-32. Hand Calculation of the PU241 β Numerator in the Two Region Slab Lattice Test

	Integrated Adjoint Flux	Delay χ	Delay υ	Fission	Integrated Forward Flux	Numerator	PERSENT
Family 1							
CORE2A	1.376E+14	0.60	0.00680	1.59303	1.173E+20	2.061E+26	2.061E+26
	1.050E+14	0.40	0.00700	1.81456	1.992E+20		
	7.069E+13	0.00	0.00720	4.26033	2.362E+19		
CORE2B	1.416E+14	0.60	0.00680	1.59303	1.258E+20	2.082E+26	2.082E+26
	1.071E+14	0.40	0.00700	1.81456	1.936E+20		
	7.457E+13	0.00	0.00720	4.26033	2.076E+19		
CORE2C	1.435E+14	0.60	0.00680	1.59303	1.297E+20	2.100E+26	2.100E+26
	1.081E+14	0.40	0.00700	1.81456	1.914E+20		
	7.626E+13	0.00	0.00720	4.26033	1.968E+19		
Family 2							
CORE2A	1.376E+14	0.80	0.00880	1.59303	1.173E+20	2.790E+26	2.790E+26
	1.050E+14	0.20	0.00900	1.81456	1.992E+20		
	7.069E+13	0.00	0.00920	4.26033	2.362E+19		
CORE2B	1.416E+14	0.80	0.00880	1.59303	1.258E+20	2.825E+26	2.825E+26
	1.071E+14	0.20	0.00900	1.81456	1.936E+20		
	7.457E+13	0.00	0.00920	4.26033	2.076E+19		
CORE2C	1.435E+14	0.80	0.00880	1.59303	1.297E+20	2.851E+26	2.851E+26
	1.081E+14	0.20	0.00900	1.81456	1.914E+20		
	7.626E+13	0.00	0.00920	4.26033	1.968E+19		

2.5.3 *Verification Using a Large Test Problem*

The previous two cases are sufficient to demonstrate that PERSENT is calculating Λ and β consistent with the stated equations in the PERSENT manual. In this last example problem, a whole core hand calculation of Λ will be done along with a single isotope β result. The same problem defined earlier in Figure 2-3 is used here. The PERSENT output excerpt of interest for this verification test is given in Figure 2-55 which corresponds to the PERSENT using the modified NHFLUX files. For Λ, one can see a contribution from every region in the problem while β of PU239 only has contributions from region C1 and C2 as that is the only place where it is located.

```
[PERSENT]...Region edits for LAMBDA
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  2.440E+21|         4.407E-09|
[PERSENT]...|ABLAN |  7.813E+21|         1.411E-08|
[PERSENT]...|RBLAN |  2.046E+22|         3.695E-08|
[PERSENT]...|CORE1 |  6.850E+22|         1.237E-07|
[PERSENT]...|CORE2 |  1.239E+23|         2.239E-07|
[PERSENT]...|ROD1A |  3.791E+21|         6.847E-09|
[PERSENT]...|ROD2A |  4.781E+21|         8.636E-09|
[PERSENT]...|ROD3A |  4.372E+21|         7.897E-09|
[PERSENT]...|ROD4A |  1.805E+21|         3.259E-09|
[PERSENT]...|ROD5A |  2.594E+21|         4.685E-09|
[PERSENT]...|ROD1B |  5.879E+20|         1.062E-09|
[PERSENT]...|ROD2B |  3.963E+21|         7.158E-09|
[PERSENT]...|ROD3B |  4.372E+21|         7.897E-09|
[PERSENT]...|ROD4B |  8.533E+20|         1.541E-09|
[PERSENT]...|ROD5B |  6.414E+19|         1.159E-10|
=PERSENT...Parameter LAMBDA Generation time  4.52146E-07 Prompt Lifetime  4.31065E-07 denom 5.53648E+29 k-eff  9.5337439E-01
[PERSENT]...Region edits for BETA PU239    family   1
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
…
[PERSENT]...|CORE1 |  1.494E+26|         2.699E-04|
[PERSENT]...|CORE2 |  3.720E+26|         6.720E-04|
…
=PERSENT...BETA PU239    family   1  9.41899E-04 denominator  5.53648E+29 k-eff  9.5337439E-01
[PERSENT]...Region edits for BETA PU239    family   2
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
…
[PERSENT]...|CORE1 |  1.351E+26|         2.440E-04|
[PERSENT]...|CORE2 |  3.362E+26|         6.073E-04|
…
=PERSENT...BETA PU239    family   2  8.51295E-04 denominator  5.53648E+29 k-eff  9.5337439E-01
[PERSENT]...Region edits for BETA cumulative PU239
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
…
[PERSENT]...|CORE1 |  2.845E+26|         5.139E-04|
[PERSENT]...|CORE2 |  7.083E+26|         1.279E-03|
…
```

Figure 2-55. Flat Flux PERSENT Output Excerpt of Λ and PU239 β for the Large Scale Test

The Λ calculation requires the domain wide forward and adjoint flux data which was obtained from PrintTables.x dumps of the RTFLUX and ATFLUX file data. The hand calculation is provided in the companion EXCEL document mentioned earlier. In the hand calculation, the hexagon average flux results in RTFLUX and ATFLUX for each energy group are combined with the velocities to produce a numerator sum of 2.50330E+23. The numerator sum is not reported in the PERSENT output but it can be calculated in two ways, the results from both are provided in Table 2-33. The italicized numbers in Table 2-33 are those taken directly from the PERSENT output while the others are hand calculated. The first approach is to sum all of the region-wise numerator results which yields 2.528E+23 for the PERSENT calculation and 2.503E+23 for the Flat Flux PERSENT calculation. Because the output data is restricted to four significant digits, the accuracy check is also limited to four significant digits. As can be seen, the hand calculation result matches the Flat Flux PERSENT result rather well. The second way to calculate the numerator

from the PERSENT output is to take the generation time and multiply by the denominator. In this case, the PERSENT calculation yields 2.52746E+23 while the Flat Flux PERSENT calculation is 2.50330E+23 which exactly matches the hand calculation to the displayed six significant digits. Using the PERSENT computed denominator, the numerator from the hand calculation can be used to produce the generation time as done in Table 2-33. The result is nearly identical to the Flat Flux PERSENT output.

Table 2-33. Hand Calculation of Λ for the Large Scale Test

	Hand Calculation	PERSENT Flat Flux	PERSENT
Denominator		*5.53648E+29*	*5.57707E+29*
Generation Time	4.52147E-07	*4.52146E-07*	*4.53188E-07*
Numerator Via Region Output Summation		*2.503E+23*	*2.528E+23*
Generation Time Denominator	2.50330E+23	2.50330E+23	2.52746E+23

From the hand calculation of Λ done here and in the previous two test problems, we can conclude that PERSENT is reliably computing Λ and doing so consistently with the equations displayed in the PERSENT manual.

Continuing with β, again the hand calculation is too lengthy to display here and is provided in the companion EXCEL document. Table 2-34 provides the details of the hand calculations where the italicized numbers are taken directly from the Flat Flux PERSENT output and the rest are hand calculated. Starting with Family 1, one can see that the hand calculated results match the Flat Flux PERSENT results but are in visible disagreement with the other PERSENT result. This is of course expected given the hand calculation can only exactly reproduce the Flat Flux PERSENT result. The total β numerator from PERSENT is calculated using the denominator and β value reported by PERSENT. As can be seen, the hand calculation is almost identical to the Flat Flux PERSENT result and only a few percent different from the other PERSENT result.

Table 2-34. Hand Calculation of β for PU239 for the Large Scale Test

		Hand Calculation	PERSENT Flat Flux	PERSENT
Denominator			*5.53648E+29*	*5.57707E+29*
Family 1	β Numerator C1	1.49432E+26	*1.494E+26*	*1.498E+26*
	β Numerator C2	3.72049E+26	*3.720E+26*	*3.748E+26*
	β Numerator	5.21481E+26	5.21480E+26	5.24577E+26
	β	9.41900E-04	*9.41899E-04*	*9.40596E-04*
Family 2	β Numerator C1	1.35082E+26	*1.351E+26*	*1.354E+26*
	β Numerator C2	3.36237E+26	*3.362E+26*	*3.387E+26*
	β Numerator	4.71318E+26	4.71318E+26	4.74089E+26
	β	8.51296E-04	*8.51295E-04*	*8.50068E-04*

Total	β Numerator C1	2.84513E+26	*2.845E+26*	*2.853E+26*
	β Numerator C2	7.08286E+26	*7.083E+26*	*7.134E+26*
	β	1.79320E-03	1.79319E-03	1.79066E-03

The Family 2 numerator results from the hand calculation exactly matches the Flat Flux PERSENT result which indicates the Family 1 detail was most likely in error due to round off error from the inputs to the hand calculation. The total β result from the hand calculation of family 2 is also nearly a perfect match to the Flat Flux PERSENT result. Again, the results are only a few percent off from the unmodified PERSENT output. The last section of Table 2-34 displays the sum of the Family 1 and Family 2 details and shows that the hand calculation is again nearly a perfect match to the modified PERSENT result. The hand calculation of β for this isotope with respect to the unmodified PERSENT result is less than 0.15%.

From the preceding hand calculations of β in this section and those before it, one can conclude that PERSENT is correctly performing the calculation of β consistent with the described equations in the PERSENT manual. In all of the above hand calculations, PERSENT was executed using modified forward and adjoint NHFLUX files to impose a flat flux approximation. This was done such that the hand calculation could match the PERSENT result where the alternatives required considerably more effort. In many cases, the modified PERSENT result was relatively similar to the unmodified PERSENT result indicating that the average value of the flux in each mesh tends to dominate the total response. In conclusion, the preceding work satisfies the verification of task a) and b) of category 4 in Table 1-1.

2.5.4 *Verification of the Effective Coalesced Parameter Representation*

The last aspect to verify is that the coalesced parameter representation is consistent with the full isotopic representation. To do this, the point kinetics equations are solved using the full isotope kinetics system and the coalesced set. Because none of this work requires any computational work from PERSENT, the work shown here is only included in the supplemental folder labeled as coalescedcheck. To demonstrate this, the point kinetics equations must be defined for the full system and the effective one, then discretized and solved for a given test case.

The point kinetics system to solve has the form

$$\frac{dp(t)}{dt} = \frac{\rho(t) - \beta}{\Lambda_G} p(t) + \sum_i \sum_m \bar{\lambda}_{i,m} C_{i,m}(t) \tag{37}$$

$$\frac{dC_{i,m}(t)}{dt} = -\bar{\lambda}_{i,m} C_{i,m}(t) + \frac{\bar{\beta}_{i,m}}{\Lambda_G} p(t). \tag{38}$$

The *i* index is for the number of fissionable isotopes and *m* is the number of delay families per fissionable isotope. The initial conditions for a given steady state power level are given as

$$C_{i,m}(0) = \frac{\beta_{i,m}}{\Lambda_G \lambda_{i,m}} p(0). \tag{39}$$

For the effective coalesced system, the *i* index is dropped from the preceding equations as there is only a single (coalesced) fissionable isotope. While it is rather easy to obtain a physically realistic set of kinetics parameters for the above equations, manufactured coefficients can be more instructive when it comes to displaying the accuracy of the coalesced approach. In this regard, the

delay family detail from Table 2-27 is augmented below in Table 2-35, Table 2-36, and Table 2-37 with manufactured β data. The first test in Table 2-35 has a consistent distribution of delayed neutrons between different families. The second test in Table 2-36 is quite unrealistic in that each isotope has a very different distribution with regard to family. In particular, Pu-239 and Pu-240 have their peak contributions to family 5 and 6 while U-235 and U-238 peaks at family 3. Finally, the third test in Table 2-37 is also unrealistic as the decay constants indicate severely different fits.

For the point kinetics equations, either table defines a discrete system with 25 unknowns to be solved for at each time point (24 precursor concentrations and 1 power). The effective coalesced kinetics parameters are easy to compute and given in Table 2-38 for all three test cases. It should be quite apparent that the decay constants do not match those appearing in Table 2-35 or Table 2-36. For the third test, the decay constant are considerably different from those in Table 2-37.

With regard to solving the point kinetics equations, there are a considerable number of methodologies in the literature. While higher order methodologies are generally preferred to discretize the point kinetics equations given their efficiency, for the verification purposes here, a simple explicit differencing approximation in time was used.

Table 2-35. Isotopic Kinetics Data for the First Coalesced Parameter Verification

Family	U-235		U-238		Pu-239		Pu-240	
	λ	β	λ	β	λ	β	λ	β
1	0.0133	1.000E-04	0.0136	6.900E-05	0.0133	1.008E-04	0.0136	3.308E-05
2	0.0327	2.750E-04	0.0313	1.717E-04	0.0309	2.269E-04	0.0300	6.737E-05
3	0.121	5.250E-04	0.123	3.174E-04	0.113	4.063E-04	0.117	1.168E-04
4	0.303	4.250E-04	0.324	2.933E-04	0.293	4.284E-04	0.307	1.406E-04
5	0.849	1.875E-04	0.906	1.269E-04	0.857	1.819E-04	0.870	5.854E-05
6	2.85	6.250E-05	3.05	4.313E-05	2.73	6.300E-05	3.00	2.067E-05

Table 2-36. Isotopic Kinetics Data for the Second Coalesced Parameter Verification

Family	U-235		U-238		Pu-239		Pu-240	
	λ	β	λ	β	λ	β	λ	β
1	0.0133	1.000E-04	0.0136	3.450E-04	0.0133	1.714E-04	0.0136	1.214E-04
2	0.0327	2.750E-04	0.0313	2.793E-04	0.0309	5.714E-05	0.0300	5.357E-05
3	0.121	5.250E-04	0.123	1.232E-04	0.113	9.143E-05	0.117	1.786E-05
4	0.303	4.250E-04	0.324	4.107E-05	0.293	2.514E-04	0.307	2.857E-05
5	0.849	1.875E-04	0.906	6.571E-05	0.857	4.800E-04	0.870	7.857E-05
6	2.85	6.250E-05	3.05	1.807E-04	2.73	3.886E-04	3.00	1.500E-04

Table 2-37. Isotopic Kinetics Data for the Third Coalesced Parameter Verification

Family	U-235		U-238		Pu-239		Pu-240	
	λ	β	λ	β	λ	β	λ	β
1	0.0133	1.000E-04	0.0399	6.900E-05	0.1197	1.008E-04	0.3591	3.308E-05
2	0.0327	2.750E-04	0.0981	1.717E-04	0.2943	2.269E-04	0.8829	6.737E-05
3	0.121	5.250E-04	0.363	3.174E-04	1.089	4.063E-04	3.267	1.168E-04
4	0.303	4.250E-04	0.909	2.933E-04	2.727	4.284E-04	8.181	1.406E-04
5	0.849	1.875E-04	2.547	1.269E-04	7.641	1.819E-04	22.923	5.854E-05
6	2.85	6.250E-05	8.55	4.313E-05	25.65	6.300E-05	76.95	2.067E-05

Table 2-38. Effective Kinetics Data for the Coalesced Parameter Verification

	First		Second		Third	
Family	λ	β	λ	β	λ	β
1	0.01340	3.029E-04	0.01349	7.378E-04	0.02975	3.029E-04
2	0.03155	7.410E-04	0.03172	6.650E-04	0.06732	7.410E-04
3	0.11860	1.365E-03	0.12019	7.575E-04	0.24288	1.365E-03
4	0.30447	1.287E-03	0.30076	7.460E-04	0.67765	1.287E-03
5	0.86632	5.548E-04	0.86014	8.118E-04	1.86788	5.548E-04
6	2.86654	1.893E-04	2.85830	7.818E-04	6.37396	1.893E-04

The explicit discretization takes the form

$$\frac{dp(t)}{dt} \approx \frac{p(t+\Delta t)-p(t)}{\Delta t} = \frac{\rho(t)-\beta}{\Lambda_G} p(t) + \sum_m \lambda_{i,m} C_{i,m}(t) \quad (40)$$

$$\frac{dC_{i,m}(t)}{dt} \approx \frac{C_{i,m}(t+\Delta t)-C_{i,m}(t)}{\Delta t} = -\lambda_{i,m} C_{i,m}(t) + \frac{\beta_{i,m}}{\Lambda_G} p(t) \quad (41)$$

This form can be cast into the matrix-vector system

$$\begin{pmatrix} p(t+\Delta t) \\ C_{1,1}(t+\Delta t) \\ \vdots \\ C_{i,m}(t+\Delta t) \end{pmatrix} = \begin{pmatrix} \frac{\rho(t)-\beta}{\Lambda_G}\Delta t + 1 & \lambda_{1,1}\Delta t & \cdots & \lambda_{i,m}\Delta t \\ \frac{\beta_{1,1}}{\Lambda_G}\Delta t & 1-\lambda_{1,1}\Delta t & 0 & 0 \\ \vdots & 0 & \ddots & 0 \\ \frac{\beta_{i,m}}{\Lambda_G}\Delta t & 0 & 0 & 1-\lambda_{i,m}\Delta t \end{pmatrix} \begin{pmatrix} p(t) \\ C_{1,1}(t) \\ \vdots \\ C_{i,m}(t) \end{pmatrix}$$

$$\xi(t+\Delta t) = M \cdot \xi(t) \quad (42)$$

This differencing approach is known to be accurate so long as the time step size is sufficiently small. From the literature, the time step should be on the order of Λ_G which highlights the downside of this methodology in that it can be extremely expensive. To avoid this, one can make use of recursive matrix-matrix products. This reduces the computational effort assuming the matrix is small and the reactivity insertion is constant (or linear) for a given macro time step. The methodology takes the following form

$$\xi(t+\Delta t) = M \cdot \xi(t)$$

$$\xi(t+2\cdot\Delta t)=M\cdot\xi(t+\Delta t)=M\cdot M\cdot\xi(t)$$
$$\xi(t+4\cdot\Delta t)=M^4\cdot\xi(t)$$
$$\xi(t+2^N\cdot\Delta t)=M_j\cdot\xi(t)$$
$$M_j=M_{j-1}\cdot M_{j-1}\quad j\in 1,N\quad M_0=M \tag{43}$$

As can be seen, the matrix needed to advance a large distance in time can be computed rather cheaply. As an example, if *N*=32, then 32 matrix-matrix multiplications are needed to compute a matrix which can transition 4,294,967,296 time steps. Assuming a value of Λ_G =10^{-7} and a time step of that size, then this would translate to a 429 second macro time step evaluation. It should be clear that a high order methodology will require on the order of 20 matrix-vector products which is considerably less expensive than the displayed approach here (32 matrix-matrix products).

The preceding matrix-matrix approach was programmed into MathCAD [11] and used to compute the solution at many intermediate time steps for all three test cases. The reactivity insertion was set as 15 pcm in all of the tests and the kinetics equations were solved up to 120 seconds (well above the longest lived half life of any precursor family). Figure 2-56, Figure 2-57, and Figure 2-58 display the power results for the first, second, and third kinetics data sets, respectively. Starting with the first test case, one can see in Figure 2-56 that the effective data set is very similar to the full system with small errors. Similarly, in Figure 2-57, the effective system is rather accurate compared with the full system for a large part of the time range. From these two results, one can conclude that the effective approach is quite accurate for isotopes that are fitted with similar decay constants but have widely varying β. The last test, Figure 2-58, shows a slight degradation in the accuracy relative to the other two test problems and the two solutions are clearly producing different results after 0.1 seconds have elapsed.

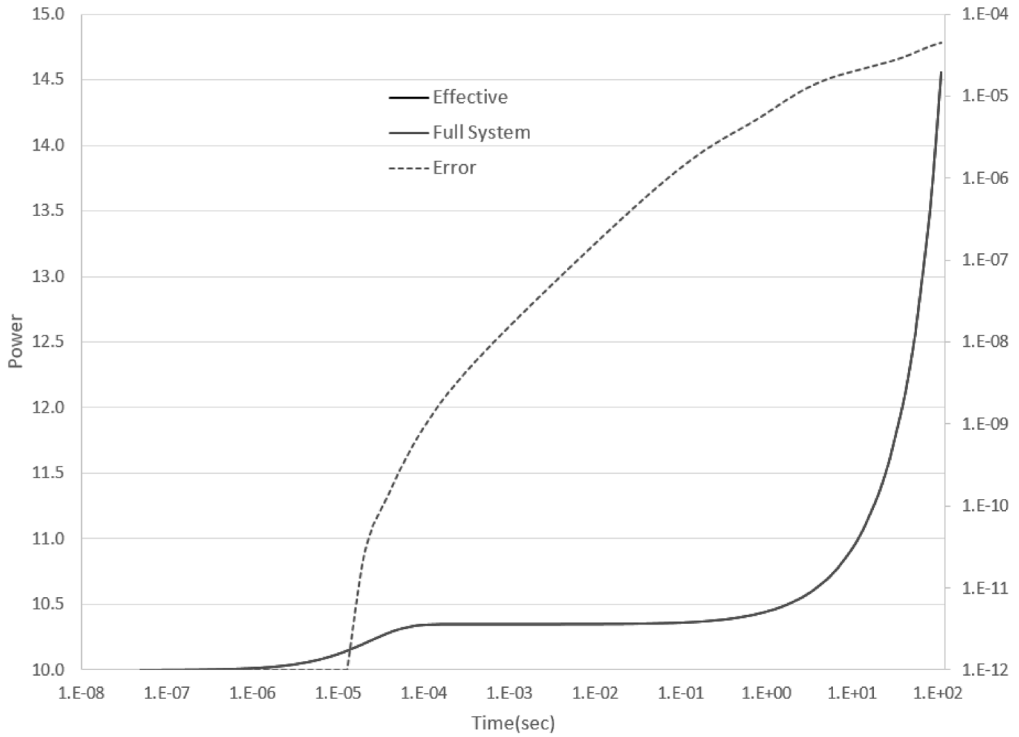

Figure 2-56. Power Result for the First Test Coalesced Parameter Verification

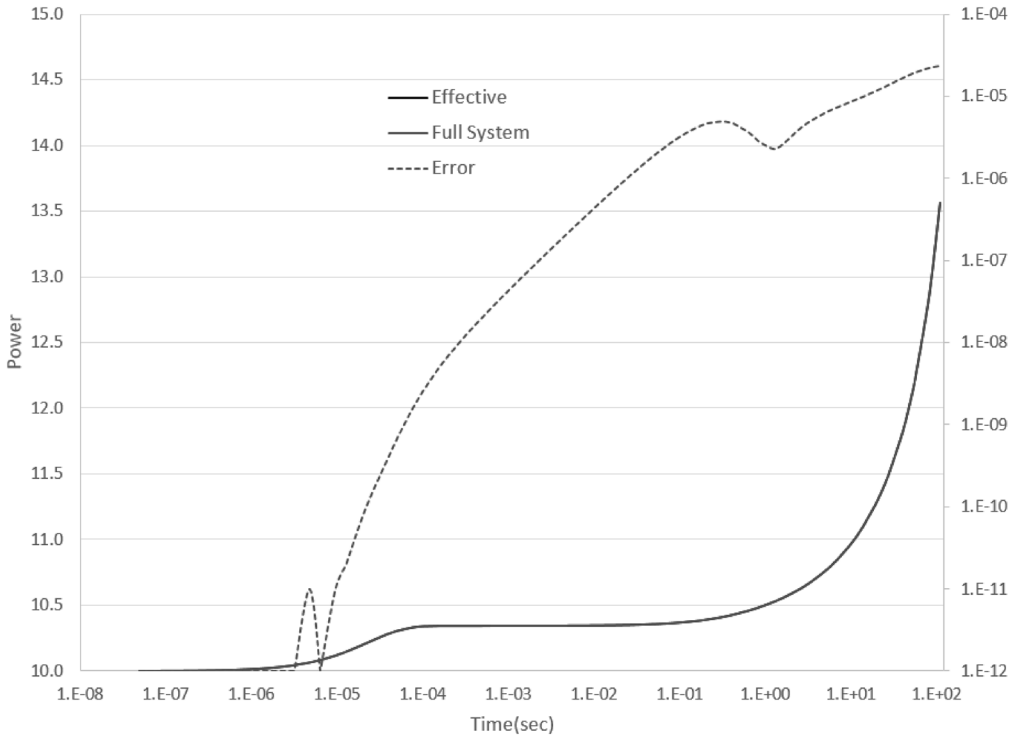

Figure 2-57. Power Result for the Second Test Coalesced Parameter Verification

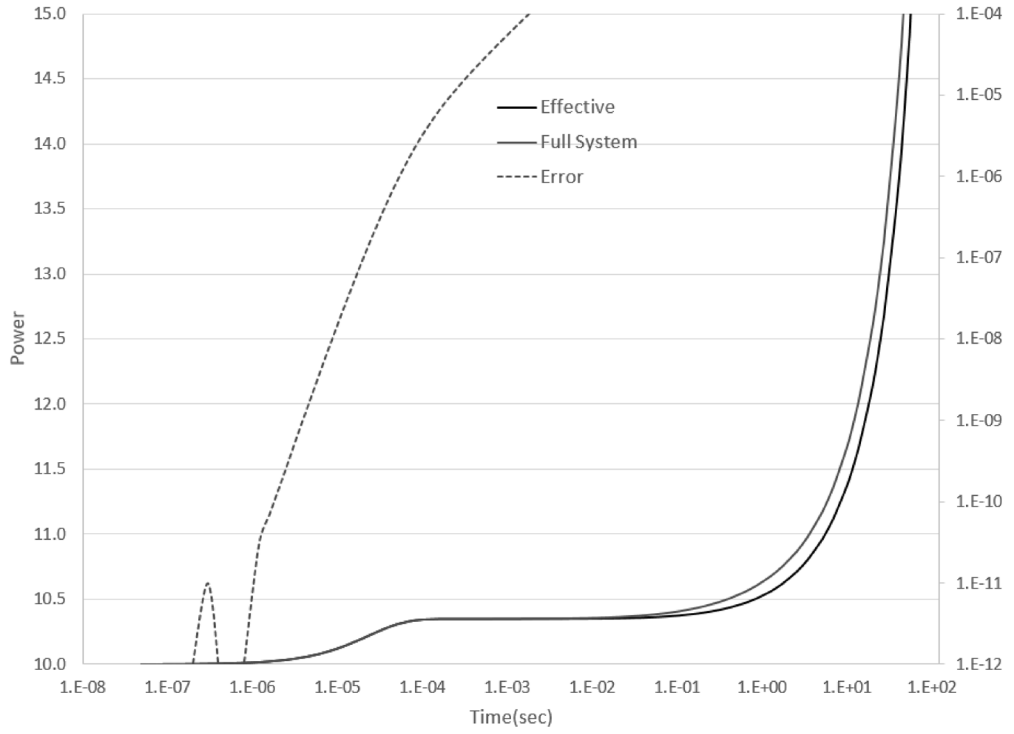

Figure 2-58. Power Result for the Third Test Coalesced Parameter Verification

While the last case does point to a potential concern for the use of the effective methodology over the full system, in reality, the decay constants used in the test are so unrealistic that one should not infer to much from this. Most of the error seen in Figure 2-56 and Figure 2-57 is attributable to the limits of double precision math and also not a concern for the methodology. From all three tests, the effective coalesced results produced by PERSENT should prove to be an effective approximation of the full set of kinetics parameters. With the preceding work displayed, task c) of category 4 in Table 1-1 is completed.

2.6 PERSENT Sensitivity Coefficient Verification

In the previous verification work, the perturbation theory related capabilites of PERSENT were checked out by a series of direct calculations with DIF3D. Manufactured problems were also used where the flux solution going into PERSENT was constrained in a way to allow a hand calculation to be carried out. For sensitivity coefficients, none of these actions will work. The essence of the sensitivity coefficient and the way it will be verified in this section is determined from equation 3.26 in the PERSENT manual as

$$s_\alpha = \frac{\alpha}{R}\frac{\partial R}{\partial \alpha} \approx \frac{\alpha}{R(\alpha)}\frac{R(\alpha + c\cdot\alpha) - R(\alpha)}{c\cdot\alpha} = \frac{R(\alpha + c\cdot\alpha) - R(\alpha)}{c\cdot R(\alpha)}. \tag{2.44}$$

In this equation, s_α is the sensitivity coefficient that PERSENT computes for the response $R(\alpha)$ to the cross section α. Equation 2.44 above displays a finite difference approximation of the sensitivity coefficient. As the PERSENT manual discusses, the sensitivity coefficients are not obtained with the displayed finite difference methodology, but by a rather complex procedure which involves knowing the derivative of the response. The responses in PERSENT that sensitivity coefficients can be generated for are collected and shown in Table 2-39. The details on each equation will be discussed in subsequent sections with the verification work on the problem along with the specifics on how the response is evaluated. From equation 2.44 above, it should be clear that the response will need to be evaluated at the base (α) and perturbed ($\alpha + c\cdot\alpha$) states.

For the reaction rate, reaction rate ratio, and power fraction response, the finite difference evaluation in equation 2.44 is not terribly difficult as it just requires using DIF3D with a perturbed cross section set to obtain a new flux solution and new evaluation of the reaction rates involved in the response. What is problematic is that DIF3D does not generate reaction rate details as part of its regular output. While the SUMMAR module does report some isotopic reaction rate summaries, they are not complete with regards to the verification work of interest here. PERSENT presently generates sensitivity coefficients for ν, χ, and Σ_x where x includes the isotopic reactions for fission (n,f), capture (n,c), elastic scattering (P_0 and P_1), inelastic scattering (P_0 and P_1) and N_2N in the standard set of sensitivity coefficients. The full output of PERSENT includes sensitivity coefficients for (n,γ), (n,α), (n,proton), (n,tritium), and (n,deuterium). To handle equation 2.44 for all reactions, a program would have to be built that can generate the response for the base state and each perturbed state. As an alternative, PERSENT reports the response of interest in its output to seven significant digits along with the corresponding sensitivity coefficients. In that regard, PERSENT can be used to obtain the perturbed response parameter given the perturbed ISOTXS file is provided to it. It should be noted that the sensitivity coefficients are not needed and that the solution of the special inhomogeneous problems can be avoided by just linking to the files needed to obtain the sensitivity coefficients in the base state.

The prompt neutron lifetime and delayed neutron fraction responses in Table 2-39 pose a similar problem to the reaction rate ones in that they are not produced by DIF3D. Instead they are produced by PERSENT in six significant digit output and thus again, PERSENT can be used with modified cross section library to obtain the perturbed state of the responses.

The eigenvalue and reactivity worth responses are more straghtforward than the previous ones as one can simply use the DIF3D eigenvalue output in the perturbed state to determine the coefficient. This of course has 8 significant digits of output where PERSENT only reported the eigenvalue with 6 significant digits in the sensitivity coefficients but 8 digits in the perturbation problems. It should be noted that the reactivity worth will require the forward and adjoint flux solutions to be obtained for both the base and perturbed state in order to get the correct finite difference result. Because the reactivity worth is a special use of the eigenvalue sensitivity, it will be verified in a different manner than all of the rest of the sensitivity coefficients.

Table 2-39. Response Functions for the PERSENT Sensitivity coefficients

Title	Response	PERSENT Manual
Reaction Rate	$\sum_g \sum_{n \in interest} \Sigma_{x,n,g} \int dV_n \int d\Omega\, \psi_{n,g}(r,\hat{\Omega})$	3.29
Reaction Rate Ratio	$\frac{\int_{interest} dV \int d\Omega \int dE\, \Sigma_x(r,\hat{\Omega},E)\psi(r,\hat{\Omega},E)}{\int_{interest} dV \int d\Omega \int dE\, \Sigma_y(r,\hat{\Omega},E)\psi(r,\hat{\Omega},E)}$	3.33
Power Fraction	$\frac{\int_{interest} dV_n \int d\Omega \int dE\, PC(r,\hat{\Omega},E)\psi(r,\hat{\Omega},E)}{\int dV \int d\Omega \int dE\, PC(r,\hat{\Omega},E)\psi(r,\hat{\Omega},E)}$	3.41
Prompt Neutron Lifetime	$\frac{\langle \psi^*, v^{-1} H\psi \rangle}{\langle \psi^*, F\psi \rangle}$	3.50
Delayed Neutron Fraction	$\frac{\underline{\psi}^{*T} \underline{\underline{F}}_{i,m} \underline{\psi}}{\underline{\psi}^{*T} \underline{\underline{F}} \underline{\psi}}$	3.55
Reactivity Worth	$\frac{\alpha}{\lambda} \frac{\underline{\psi}^{*T} \frac{\partial \underline{\underline{B}}(\alpha,\lambda)}{\partial \alpha} \underline{\psi}}{\underline{\psi}^{*T} \underline{\underline{F}} \underline{\psi}} - \frac{\alpha}{\hat{\lambda}} \frac{\hat{\underline{\psi}}^{*T} \frac{\partial \hat{\underline{\underline{B}}}(\alpha,\hat{\lambda})}{\partial \alpha} \hat{\underline{\psi}}}{\hat{\underline{\psi}}^{*T} \hat{\underline{\underline{F}}} \hat{\underline{\psi}}}$	3.65
k_{eff}	$\frac{\alpha}{\lambda} \frac{\underline{\psi}^{*T} \frac{\partial \underline{\underline{B}}(\alpha,\lambda)}{\partial \alpha} \underline{\psi}}{\underline{\psi}^{*T} \underline{\underline{F}} \underline{\psi}}$	3.65

From the above, it should be clear that using PERSENT to obtain the perturbed state evaluation of the response is the wisest approach as it does not require the additional creation and verification of a program to generate those parameters. Because the output precision of PERSENT is known, this means the cross sections must be modified by a sufficient amount to actually yield a value that will produce an accurate result for equation 2.44. Because PERSENT produces sensitivity coefficients for each reaction of each isotope in the base state, this information can be used to determine the cross section perturbation that will guarantee a large enough change in the PERSENT output to get a finite difference coefficient. At issue again is the number of significant

digits of output provided by PERSENT. For everything but the eigenvalue (discussed above), the power fraction, and the reaction rate ratio sensitivities, PERSENT provides 7 significant digits of output on the response. For the eigenvalue it was 6, the power fraction is typically 4 or 5, and the reaction rate ratio is less than 7. The last two are issues because they were not displayed in PERSENT using exponential format and thus as the response goes to zero, the number of significant digits goes to zero. To remedy this, PERSENT was updated to display all of the numbers with 8 significant digits of output for the eigenvalue and 9 significant digits of output for all other responses in exponential format. This decision was made as there are so few users, a change of this type at this time makes no real difference but it does greatly improve the confidence in the verification work.

Equation 2.44 above is redefined as shown below to carry out the finite difference evaluation.

$$R(c \cdot \alpha) = R(\alpha + (c-1) \cdot \alpha) = r \cdot R(\alpha) \tag{2.45}$$

$$s_\alpha \approx \frac{\alpha}{R(\alpha)} \frac{R(\alpha + (c-1) \cdot \alpha) - R(\alpha)}{(c-1) \cdot \alpha} = \frac{r-1}{c-1} \tag{2.46}$$

$$c = 1 + \frac{r-1}{s_\alpha} \tag{2.47}$$

In equation 2.46, the sensitivity coefficient is represented as the fractional change in the response (r) divided by the fractional change in the cross section (c). From the earlier definition of the number of significant digits in the PERSENT response outputs, clearly a change in the ninth significant digit of the response will yield a zero sensitivity coefficient. Thus if PERSENT computes a sensitivity coefficient (s_α) of 10^{-9} and we want to observe a 10^{-6} change in the response (r), the cross section change (c) is found to be 1001. This is an extremely large perturbation to the cross section and the present version of ISOTXS_Modify does not allow the factor to be greater than 100. Because the factor of 100 was chosen wisely, getting a 10^{-6} change in the response is not going to be possible for very small cross section reactions like this. For sensitivity coefficients that are 10^{-2}, the cross section change (c) will be 1.0001. In both of these examples, it should be clear that the magnitude of the perturbation in the response can be kept small such that it should be in the linear regime although in some cases it will register as a zero sensitivity coefficient instead of the one computed by PERSENT. This aspect will be dealt with as it is identified to occur in the following sections.

All of the sensitivity coefficients can be generated using a single DIF3D input. Because this is a verification task, that input should have enough isotopes to be a true test of the PERSENT capabilities. Because the reaction rate sensitivity requires the model be sub-critical in the base state and all perturbations, that is another constraint when defining the DIF3D model. Benchmarks 8 and 15 in the PERSENT verification test suite are well suited to the current testing as it contains many isotopes consistent with modern reactor analysis and is not computationally intensive. Benchmark 15 was detailed in section 6.2 of the PERSENT manual and the geometry and flux distribution are reproduced here in Figure 2-59. The base configuration of this model has a diffusion eigenvalue of 1.04196 which is clearly not sub-critical as is required for the current work. To correct this aspect, the control rods which were parked above the active core were inserted into the active core to give diffusion and transport eigenvalues of 0.97664 and 0.99044, respectively.

To accommodate the reaction rate, reaction rate ratio, and power fraction aspects of a PERSENT sensitivity calculation, special isotopes and regions need to be defined in the domain so they can be selected. Figure 2-60 provides the ISOTXS isotope names and their mapping to unique MC^2 isotope library names that PERSENT uses as part of the sensitivity coefficients. The various ISOTXS isotopes that end in Z were all added to accommodate the needs of these sensitivity calculations. For the reaction rate sensitivity, a contaminant of U-233 (U233Z) was assumed in all positions of the radial reflector which is highlighted in red font in the DIF3D input excerpt shown in Figure 2-61. This is of course not realistic, but is an appropriate test of the reaction rate sensitivity calculation. U-233 was chosen as it does not appear anywhere else in the domain.

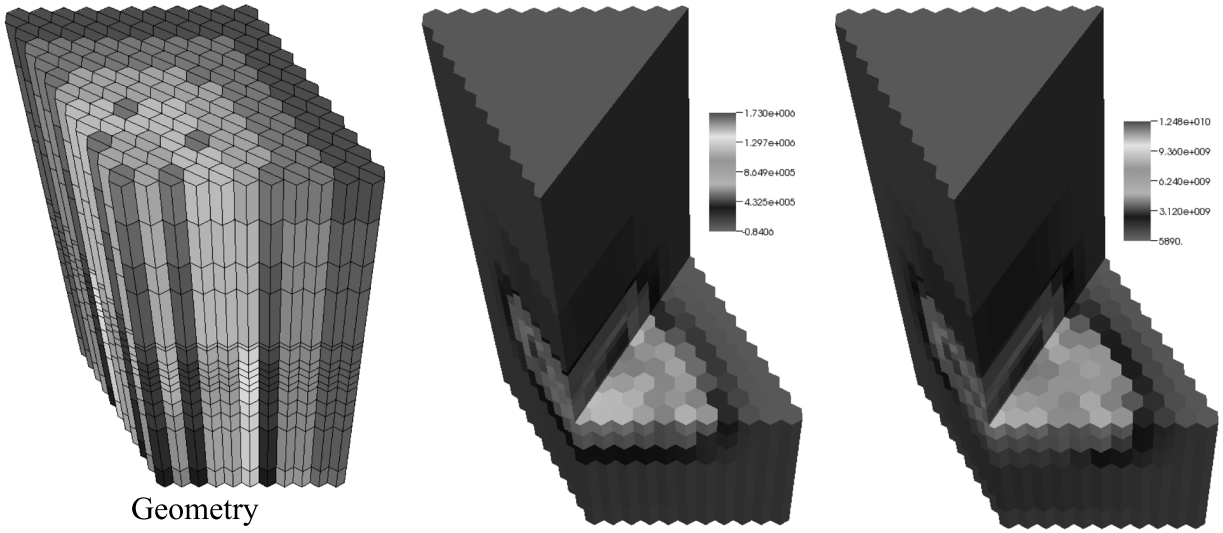

Figure 2-59. The Geometry and Group 6 Flux Distributions for Verification Test #15.

```
Index Unique  ISOTXS ->
    1 AM2415  A241I    A241M    A241O
    2 AM2425  A242I    A242M    A242O
    3 AM243V  A243I    A243M    A243O
    4 AM242M  A24MI    A24MM    A24MO
    5 B-105   B-10I    B-10M    B-10O    B-10S
    6 B-115   B-11I    B-11M    B-11O    B-11S
    7 C-125   C-12I    C-12M    C-12O    C-12S
    8 CM2415  C241I    C241M    C241O
    9 CM2425  C242I    C242M    C242O
   10 CM2435  C243I    C243M    C243O
   11 CM2445  C244I    C244M    C244O
   12 CM2455  C245I    C245M    C245O
   13 CM2465  C246I    C246M    C246O
   14 CRS     CRI      CRM      CRO      CRR      CRS
   15 HOMOG   DUMP1    DUMP2
   16 FESV    FEI      FEM      FEO      FER      FES
   17 HE45    HE-4
   18 LFP35   LFP35
…
   23 MN555   MN55I    MN55M    MN55O    MN55R    MN55S    MN55Z
   24 MO5     MOI      MOM      MOO      MOR      MOS
   25 N-145   N-14I    N-14M    N-14O
   26 NP237V  N237I    N237M    N237O
   27 NP2385  N238I    N238M    N238O
   28 NA23S   NA23I    NA23M    NA23O    NA23R    NA23S
   29 NIS     NII      NIM      NIO      NIR      NIS
   30 O-165   O-16I    O-16M    O-16O
   31 PA2335  P233I    P233M    P233O    P233Z
   32 PU2365  P236I    P236M    P236O    P236Z
   33 PU2375  P237I    P237M    P237O    P237Z
   34 PU2385  P238I    P238M    P238O    P238Z
   35 PU239V  P239I    P239M    P239O    P239Z
   36 PU2405  P240I    P240M    P240O    P240Z
   37 PU2415  P241I    P241M    P241O    P241Z
   38 PU2425  P242I    P242M    P242O    P242Z
   39 PU2435  P243I    P243M    P243O    P243Z
   40 PU2445  P244I    P244M    P244O    P244Z
   41 TH2325  T232I    T232M    T232O    T232Z
   42 U-2335  U233I    U233M    U233O    U233Z
   43 U-2345  U234I    U234M    U234O    U234Z
   44 U-2355  U235I    U235M    U235O    U235Z
   45 U-2365  U236I    U236M    U236O    U236Z
   46 U-2375  U237I    U237M    U237O    U237Z
   47 U-2385  U238I    U238M    U238O    U238Z
   48 ZRSV    ZIRCI    ZIRCM    ZIRCO    ZIRCR
```

Figure 2-60. PERSENT Output Excerpt of ISOTXS Isotope Mapping to Unique MC^2 Names

```
30    RF9_A      8     0     0        0.0        35.76
30    RF9_G      8     0     0       35.76      435.50
30    RF9RR      8     3     3      194.12      217.11
30    RF9_K      8     0     0      435.50      480.20
30     RF0_A     9     0     0        0.0        35.76
30     RF0_G     9     0     0       35.76      435.50
30     RF0_K     9     0     0      435.50      480.20
14    RF9_A FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14    RF9_A CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
14    RF9_A U233Z  1.0E-7
14     RF9_G FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14     RF9_G CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
14     RF9_G U233Z  1.0E-7
14    RF9RR FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14    RF9RR CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
14    RF9RR U233Z  1.0E-7      MN55Z  2.0E-7
14    RF9RR T235Z  1.0E-7      U238Z  1.0E-7      P239Z  1.0E-7
14     RF9_K FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14     RF9_K CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
14     RF9_K U233Z  1.0E-7
14    RF0_A FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14    RF0_A CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
14     RF0_G FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14     RF0_G CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
14    RF0_K FER    5.89102E-02 NA23R  3.45173E-03 MOR    4.14113E-04
14    RF0_K CRR    8.75918E-03 NIR    3.63219E-04 MN55R  3.88047E-04
15  RF9_A RF9_A
15  RF9_G RF9_G
15  RF9RR RF9RR
15  RF9_K RF9_K
15    RF0_A RF0_A
15    RF0_G RF0_G
15    RF0_K RF0_K
```

Figure 2-61. Excerpt of the DIF3D Input to Accommodate Reaction Rate Sensitivities

For the reaction rate ratio sensitivity, foil cross sections for Pu-239 (P239Z), Th-235 (T232Z), U-238 (U238Z), and Mn-55 (MN55Z) were added to a single axial mesh in the radial reflector

which is highlighted in blue font in Figure 2-61. The affected mesh is in ring 8 at position 3 and axially between 194.12 cm and 217.11 cm. Because of the way the spatial integral is done in the reaction rate ratio evaluation, the reaction rate ratio will effectively be at the centroid of this mesh. Reaction rate ratios of U-238 capture over Pu-239 fission are considered along with Th-232 capture over Mn-55 capture. The latter of these was chosen as Th-232 is not present anywhere else in the domain and it should have a very strong component to the sensitivity. For power fraction, two new regions were added to the model in ring 4 at position 3 between 148.15 cm and 194.12 cm. This sensitivity coefficient does not need isotopic manipulation and thus no additional information is needed.

With these changes to the base DIF3D model, one should understand that all of the sensitivity coefficients for all responses in Table 2-39 can be obtained using a single PERSENT input. This is the approach taken where benchmark 32 is for diffusion theory and benchmark 33 is for transport. Figure 2-60 shows the PERSENT input for both cases but only the output from the diffusion theory result is detailed here for brevity. The reaction rate, reaction rate ratio, and power fraction sensitivity coefficients will be very large on the reactions of those isotopes included in the reaction and the finite difference calculations will have to be specific to each sensitivity coefficient.

```
FORCE_FULL_FLUX     YES
DIF3D_EXECUTABLE    dif3d.x
DIF3D_INPUT         dif3d.base.inp
ISOTXS_INPUT        user.ISOTXS

LAMBDA_BETA      YES

SENSITIVITY_KEFF  ReferenceCore
SELECT_ALPHA      ReferenceCore  IGNOREIT   everything

ISOTOPE_LIST   RTargetI U233Z
ZONE_LIST      RTargetZ RF9_A RF9_G RF9RR RF9_K
REACTION_RATE  ReactionU233  RTargetI gamma RTargetZ
SELECT_ALPHA   ReactionU233  IGNOREIT   everything

ISOTOPE_LIST    RRTargetN1 P239Z
ISOTOPE_LIST    RRTargetD1 U238Z
ZONE_LIST       RRTargetZ  RF9RR
REACTION_RATIO  RR_fP239_cU238  RRTargetN1 fission RRTargetZ   RRTargetD1 capture RRTargetZ
SELECT_ALPHA    RR_fP239_cU238  IGNOREIT   everything

ISOTOPE_LIST    RRTargetN2 T232Z
ISOTOPE_LIST    RRTargetD2 MN55Z
ZONE_LIST       RRTargetZ  RF9RR
REACTION_RATIO  RR_cT232_fP239  RRTargetN2 capture RRTargetZ   RRTargetD2 capture RRTargetZ
SELECT_ALPHA    RR_cT232_fP239  IGNOREIT   everything

ZONE_LIST       PFTargetZ  MC5XD MC5XE
POWER_FRACTION  PF_MC53DE  PFTargetZ
SELECT_ALPHA    RR_cT232_fP239  IGNOREIT   everything

SENSITIVITY_BETA BetaBetaBeta

SENSITIVITY LAMBDA LambdaLambda
```

Figure 2-62. PERSENT Input for Generating Sensitivity Coefficients

2.6.1 *Verification of the PERSENT Eigenvalue Sensitivity Coefficients*

The first verification test problem is benchmark 32 in the PERSENT distribution and covers the eigenvalue response in Table 2-39. The full PERSENT input and output are detailed here for completeness but it

Because the DIF3D calculations can be completed more efficiently using a restarted flux solution from DIF3D, the perturbed state PERSENT calculations will all use external NHFLUX and NAFLUX files for both the base and perturbed states. Since the cross sections from ISOTXS used by DIF3D are slightly different in diffusion theory versus transport,

2.1 PERSENT Uncertainty Quantification Verification

The first verification test pr

3 Summary of the Preceding Verification Work

The preceding work verified categories 1 through 4 of Table 1-1. Category 5 verification will be added at a later date and will be a version update to this report. The set of test problems is summarized in Table 3-1 along with cross referencing for the section of this report it is discussed in and the category that it satisfies.

Table 3-1. Verification Test Problems and Cross Referencing to Category and Section.

PERSENT Index ID	DIF3D Index ID	Verification Section	Verification Category
20	42	2.1.1	1. a) b)
21	43	2.1.2	1. a) b) 2. a)
22	44	2.2.1	2. a)
23	45	2.2.2 2.2.3	2. a) b)
24	46	2.2.4	2. a) b)
25	47	2.2.5	2. c) d)
26	48	2.3	3. a) b) c)
27	49	2.5.1 2.5.2 2.5.3	4. a) b)
30		2.4	3. d)
31		2.2.6	2. e)
coalescedcheck		2.5.4	4. c)

In this document, the verification work was displayed for the perturbation theory and kinetics capabilities of PERSENT. For all identified PERSENT outputs, the work covered in this report demonstrated that the equations the PERSENT manual states are being used are consistent with the input and output of PERSENT. It is noted that the DIF3D verification report [3] ensures the accuracy of the DIF3D solution [4-9] that PERSENT relies upon.

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