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ANL/NSE-24/80

Requirements Description of the PERSENT Software

Nuclear Science and Engineering Division

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Requirements Description of the PERSENT Software

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1 Introduction

This report presents 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 identified capabilities will be used to establish the set of PERSENT verification tasks necessary to verify PERSENT for usage on commercial projects. A similar path was followed for the REBUS [2] and DIF3D [3] software packages.

One of the most well used methods currently employed for reactor analysis is the diffusion approximation. This approximation is typically employed at the whole-core level using homogenized assembly cross sections in a nodal framework as is the case in the DIF3D code [3-6] developed at Argonne National Laboratory. Perturbation theory methods have been developed for a wide range of applications in reactor analysis [7-17] many of which are still widely used for reactivity and sensitivity coefficient calculations. The reactivity change (i.e., change in the eigenvalue of the neutron transport equation) due to perturbations introduced in the system can be expressed by a conventional perturbation equation which requires a combination of the unperturbed or perturbed forward flux and the unperturbed or perturbed adjoint flux. The solution to the perturbation equation provides the contribution of a given perturbation to the reactivity change for the entire phase space of the transport equation (space, angle, and energy). The perturbation theory capability is primarily used to spatial distributions of the perturbation usable as reactivity coefficients in point kinetics safety analysis or the more simplified asymptotic analysis.

PERSENT was developed by Argonne in 2012 and released in 2013 as a replacement for the Argonne developed VARI3D [18] software. VARI3D was developed in the mid 1980s and was primarily used since to generate reactivity coefficients for safety analysis. The VARI3D software was built around the DIF3D-FD solver which was limited to diffusion theory and triangular-z meshing in hex geometries. 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. Even the sensitivity capability in VARI3D was limited to the 2D R-Z diffusion theory option of DIF3D-FD. 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 and thus a very acceptable replacement for the DIF3D-FD solver. 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

goal of this manuscript is to discuss the capabilities of the PERSENT code that are used by the commercial reactor projects that need to be verified.

2 Specific Usage of the PERSENT Software

The PERSENT software is part of the ARC (Argonne Reactor Code) system [19] and is the primary perturbation and sensitivity analysis capability. Figure 1 shows the present connections of PERSENT in the ARC system noting that it is a necessary component if the overall goal is to perform safety analysis of a proposed reactor design. The breakdown in identifying the critical engineering outputs of the PERSENT software that must be verified starts by looking at which outputs from PERSENT are being used by the analysts in the design process. The PERSENT software can be considered as two tasks: perturbation and sensitivity.

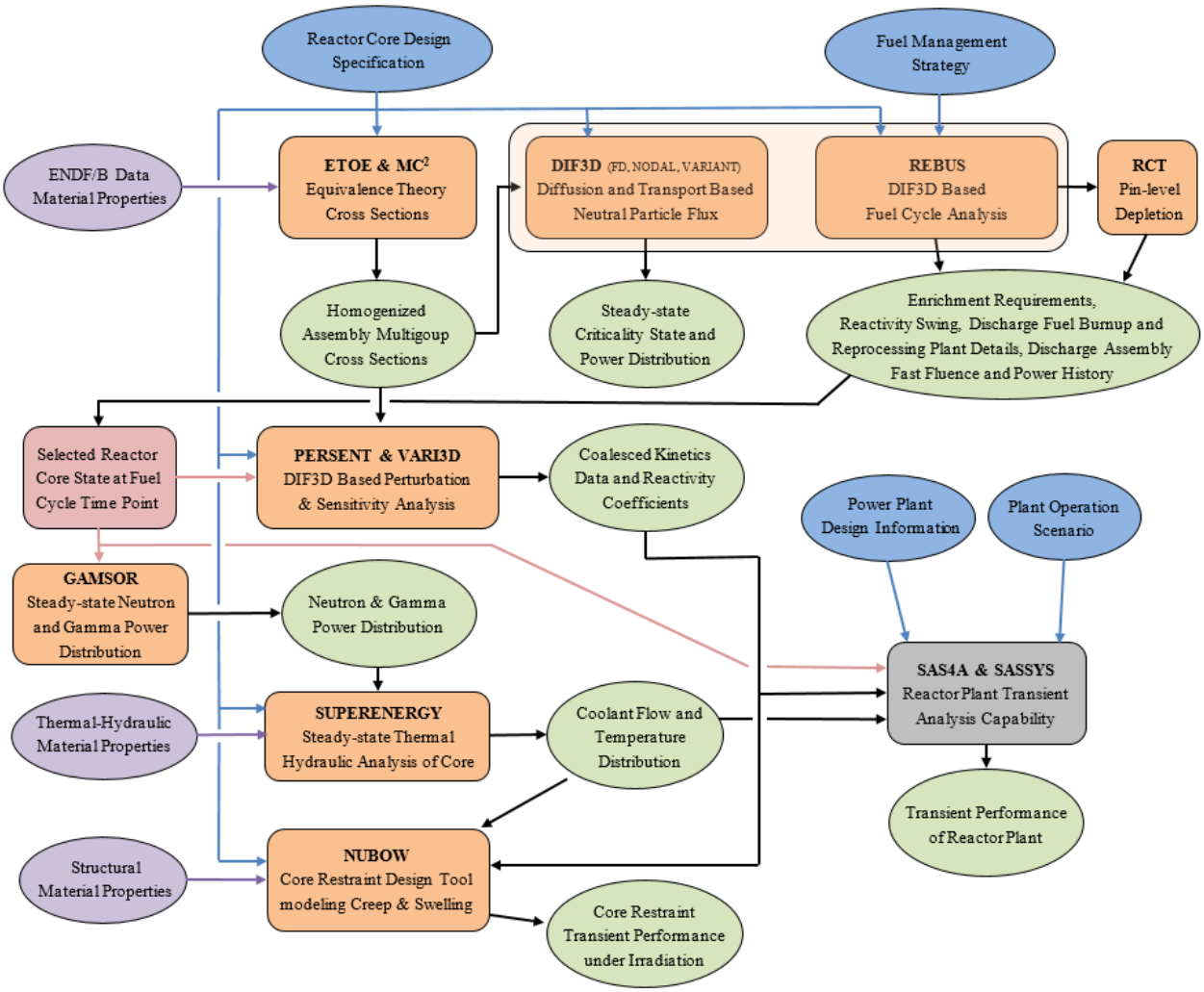

Figure 1. The Argonne Reactor Code System Set of Connected Codes

For perturbation theory uses, PERSENT presently allows the user to define cross section, density, and zone perturbations. The cross section perturbation is focused on the reactivity worth of specific cross section changes and is typically not used by reactor analysis projects. The density perturbation allows the user to determine the reactivity worth of adjusting the density of all isotopes in a zone and is also not typically used by reactor analysis projects. The zone perturbation option allows users to compute the worth of changing the contents of a zone and is used exclusively

by reactor analysis projects for generating reactivity coefficients. Exact and first order perturbation theory options are used extensively in the safety analysis work and thus both options of the zone perturbation capability must be verified.

The sensitivity coefficient calculation is not directly included in the safety analysis work for reactor projects. Instead, it is used as part of the validation work where the uncertainty quantification (UQ) methodology built into PERSENT makes use of the sensitivity coefficients. The cross section data has fundamental uncertainties in it and the purpose of the UQ analysis is to assess how much error in a given prediction of a measured quantity (burnup, control rod worth, etc…) is due to the cross section errors. The sensitivity coefficient calculation is thus a part of the process to define the uncertainty of the reactivity coefficients used in the safety analysis work. PERSENT can compute sensitivities on β, Λ, k_{eff}, reactivity worth, reaction rate ratio, reaction rate, and power fraction for a given reactor model. There are notable restrictions on the reactor rate sensitivity coefficient option. Most reactor analysis projects primarily focus on k_{eff} and reactivity worth sensitivities as these are used in the safety analysis work. The various other sensitivities are primarily needed when comparing the ARC calculated results to experimental measurements and thus are needed, but not as prominently as the first two.

Given the sensitivity coefficient data and a user provided co-variance matrix, PERSENT can perform an uncertainty quantification and representativity calculation which are additional capabilities that must be verified as part of this work.

2.1 PERSENT Inputs and Outputs to Verify

All of the PERSENT input options are compactly provided in Figure 2. A detailed description of each input can be found in the user manual [1] and is not necessary here. From the preceding discussion, the inputs from Figure 2 that will not be verified is considerably shorter than the ones that must be verified. The unverified input options include: adjust_xs, adjust_density, reaction_rate, and power_fraction. All of the other input options shown in Figure 2 must be verified as part of this work.

PERSENT is organized to consider multiple problems in the calculation process. The user can therefore provide multiple reactivity coefficient inputs along with inputs to calculate sensitivity and UQ results. Internally, PERSENT completes all perturbation theory options first followed by sensitivity and UQ calculations. The only exception is when a sensitivity calculation of a perturbation is requested for which PERSENT only performs the perturbation theory calculation as part of the sensitivity calculation process. From this setup, the output follows the problem execution and thus all output for a given perturbation or sensitivity problem appears in exactly one contiguous section of the output.

Figure 3 through Figure 5 show output excerpts of the PERSENT zone perturbation theory capability. As can be seen, the output includes a description of the problem, some details on what the storage name of the problem is followed by a mesh wise breakdown of the reactivity worth and a region-wise breakdown of the reactivity worth. The mesh wise breakdown follows the GEODST I,J,K grid representation of a 3D DIF3D geometry.

```
FORCE_FULL_FLUX  <yes/no>
ISOTXS_INPUT     <file_name>
DLAYXS_INPUT     <file_name>
DIF3D_INPUT      <file_name>
DIF3D_EXECUTABLE <file_name>
FORWARD_FILE     <file_name>
ADJOINT_FILE     <file_name>
ISOTOPE_LIST     <name_of_list> <ISOTXS isotope> <ISOTXS isotope> <ISOTXS isotope> <ISOTXS isotope> ...
ZONE_LIST        <LIST_ZONES>  <DIF3D zone> <DIF3D zone> <DIF3D zone> <DIF3D zone> ...
NEW_ZONE         <new DIF3D zone name> <ISOTXS isotope> <ISOTXS density> <ISOTXS isotope> <ISOTXS density> ...
SET_DELAY        <ISOTXS isotope> <DLAYXS isotope>
BOWING_ZONE_MAP  <original input zone> <by-pass gap zone>
BOWING_NULLIFY   <Ring or I> <Position or J>   In Cartesian(I,J) and hexagonal(Ring,Position)
------------------
LAMBDA_BETA      <no/yes>
ADJUST_XS         <problem_name> <METHOD> <ISOTOPE_LIST> <XS> <multiplicative factor> <add on factor> <start group> <end group>
ADJUST_DENSITY    <problem_name> <METHOD> <existing DIF3D zone> <density multiplicative factor>
ADJUST_ZONE       <problem_name> <METHOD> <existing DIF3D zone> <replacement zone> [density multiplicative factor]
ADJUST_GENERIC    <problem_name> <METHOD> <DIF3D input that defines the perturbed state>
BOWING_WORTH      <PROBLEM_NAME> <Neutronics starting Z position> <Duct Outer FTF> <Perturbed Strain file> [Base Strain file]
PROBLEM_EDITS     <problem_name> <PRINT_BY_: ISOTOPE, MESH, GROUP, REGION, AREA, MASS, UNIQUE, FAMILY> <PRINT_BALANCE> <EXPORT_VTK> <file_name>
FORWARD_PERT_FILE <problem_name> <file_name>
ADJOINT_PERT_FILE <problem_name> <file_name>
------------------
REACTION_RATE       <problem_name>  <ISOTOPE_LIST> <XS> <LIST_ZONES>
REACTION_RATIO      <problem_name>  <numer. ISOTOPE_LIST> <XS> <LIST_ZONES> <denom. ISOTOPE_LIST> <XS> <LIST_ZONES>
REACTION_WORTH      <problem_name>  <perturbation PROBLEM_NAME>
POWER_FRACTION      <problem_name>  <numerator LIST_ZONES>
SENSITIVITY_BETA    <problem_name>
SENSITIVITY_LAMBDA  <problem_name>
SENSITIVITY_KEFF    <problem_name>
SENSITIVITY_FILE    <problem_name>  <file name>
SENSITIVITY_DIFF    <problem_name>  <Sensitivity problem name 1> <Sensitivity problem name 2> [f1] [f2]
BILINEAR            <problem_name>  <Sensitivity problem name 1> <Sensitivity problem name 2>
SELECT_ALPHA        <problem_name>  <ISOTOPE_LIST> <XS>
SENSITIVITY_EDITS   <problem_name>  <PRINT_PERTURBATION> <PRINT_BY_ISOTOPE> <PRINT_BY_ZONE> <PRINT_BY_AREA> <file_name>
SENSITIVITY_DOUQ    <problem_name>  <Print Reaction-wise table?> <Print Detailed Isotope table?> <Print Isotope to Isotope Table?>
GAMMA_FORWARD_FILE  <problem_name>  <file_name>
GAMMA_ADJOINT_FILE  <problem_name>  <file_name>
LIMIT_OUTERS        <min iterations> <max iterations>
USE_SHIFT           <no/yes>
USE_TOTALNU         <no/yes>
TREAT_UNIQUE        <ISOTXS isotope> <ISOTXS isotope> ...  These isotopes will be uniquely treated in the sensitivity calculations
------------------
COMMARA_INPUT     <file_name>
COMMARA_IGNOREMISSINGDATA <no/yes>
COMMARA_ISOTOPE   <ISOTXS isotope> <COMMARA isotope>
COMMARA_REACTION  <PERSENT reaction> <COMMARA reaction>
------------------
<METHOD> = <FIRST_ORDER_PT> <EXACT_PT> <GENERALIZED_PT> <NS_FIRST_ORDER>
<XS> = <TOTAL> <NU> <NUFISSION> <CHI> <CHI_FD> <FISSION> <CAPTURE> <GAMMA> <ALPHA> <PROTON> <TRITIUM> <DEUTERIUM>
       <SCATTER> <ELASTIC> <INELASTIC> <N2N> <P1SCATTER> <P1ELASTIC> <P1INELASTIC> <P1N2N> <STANDARDSET> <EVERYTHING>
```

Figure 2. PERSENT Quick Guide Input Commands

```
[PERSENT]..........................................................................
[PERSENT]...Problem RC_TO_RD         is a zone perturbation using GENERALIZED_PT
[PERSENT]...Associated DIF3D output is P_dif3d_problem0001.out
[PERSENT]..........................................................................
[PERSENT]...Replacing zone     RC       with copy of zone     RD
[PERSENT]...Running DIF3D to get the perturbed forward solution
[PERSENT]...Performing the DIF3D-VARIANT numerator/denominator operations
[PERSENT]...Start of numerator/sum(denominator) table for General PT of RC_TO_RD
               1          2          3          4          5          6          7          8
    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
    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
    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
     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
     8 -7.553E-03  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.560E-03
     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
     6  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.180E-02  0.000E+00  0.000E+00
     5  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  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  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  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 -2.031E-02  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -7.553E-03
[PERSENT]...Region edits for General PT of RC_TO_RD
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission  + Out Scatt
[PERSENT]...|      |           | Sum[Denominator] |          |          |          |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E
[PERSENT]...|BLAN  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E
[PERSENT]...|CORE2 |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00|    0.000E
[PERSENT]...|ROD1  | -3.032E+19|        -2.031E-02| 2.627E-05|-1.857E-02| 0.000E+00|   -1.107E
[PERSENT]...|ROD2  | -1.127E+19|        -7.553E-03| 1.844E-03|-8.502E-03| 0.000E+00|   -5.226E
[PERSENT]...|ROD3  | -2.329E+18|        -1.560E-03| 1.242E-03|-2.485E-03| 0.000E+00|   -1.495E
[PERSENT]...|ROD4  | -3.254E+19|        -2.180E-02| 1.405E-03|-2.140E-02| 0.000E+00|   -1.325E
[PERSENT]...|ROD5  | -1.127E+19|        -7.553E-03| 1.844E-03|-8.502E-03| 0.000E+00|   -5.226E
=PERSENT...Parameter General PT of RC_TO_RD          is -5.87771E-02 denominator  1.49276E+21
…
```

Figure 3. Example PERSENT Zone Reactivity Worth Output

```
[PERSENT]..........................................................................
[PERSENT]...Problem C2_TO_C1P        is a zone perturbation using GENERALIZED_PT
[PERSENT]...Associated DIF3D output is P_dif3d_problem0003.out
[PERSENT]..........................................................................
[PERSENT]...Replacing zone     C2       with copy of zone     C1P
[PERSENT]...This perturbation has total core changes in mass of
[PERSENT]...NA23 5            -4.5737 kg
[PERSENT]...O-16 5             5.8341 kg
[PERSENT]...PU239S           -31.7057 kg
[PERSENT]...U-238S            78.9321 kg
[PERSENT]...Start of numerator/sum(denominator) table for mass(kg) change for C2_TO_C1P
…
[PERSENT]...Axial plane      7 data for mass(kg) change for C2_TO_C1P
                1          2          3          4          5          6          7          8
    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
    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
    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
     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
     8  0.000E+00  5.051E-01  5.051E-01  5.051E-01  5.051E-01  5.051E-01  5.051E-01  0.000E+00
     7  2.525E-01  5.051E-01  5.051E-01  5.051E-01  5.051E-01  5.051E-01  5.051E-01  5.051E-01
     6  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.051E-01  5.051E-01
     5  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.051E-01  5.051E-01
     4  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.051E-01  5.051E-01
     3  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.051E-01  5.051E-01
     2  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.051E-01  5.051E-01
     1  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  2.525E-01  0.000E+00
…
[PERSENT]...Region edits for mass(kg) change for C2_TO_C1P
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
…
[PERSENT]...|CORE2 |  0.000E+00|         4.849E+01|
…
[PERSENT]...|ROD5  |  0.000E+00|         0.000E+00|
=PERSENT...Parameter mass(kg) change for C2_TO_C1P    is  4.84867E+01 denominator  0.00000E+00
…
```

Figure 4. Example PERSENT Zone Reactivity Worth Output for Isotopic Mass Changes

```
…
=PERSENT...Parameter General PT of C2_TO_C1P          is -4.34583E-02 denominator
[PERSENT]...Start of numerator/sum(denominator)/mass(kg) table for General PT of
[PERSENT]...Axial plane      1 data for General PT of C2_TO_C1P
…
[PERSENT]...Axial plane      7 data for General PT of C2_TO_C1P
               1          2          3          4          5          6          7          8
    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
    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
    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
     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
     8  0.000E+00 -1.144E-03 -1.086E-03 -9.507E-04 -7.623E-04 -5.504E-04 -3.283E-04  0.000E+00
     7 -1.939E-03 -2.005E-03 -1.925E-03 -1.675E-03 -1.331E-03 -9.952E-04 -6.274E-04 -3.283E-04
     6  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -9.952E-04 -5.504E-04
     5  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.331E-03 -7.623E-04
     4  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.675E-03 -9.507E-04
     3  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.925E-03 -1.086E-03
     2  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -2.005E-03 -1.144E-03
     1  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00 -1.939E-03  0.000E+00
…
[PERSENT]...Region edits/mass(kg)  for General PT of C2_TO_C1P
[PERSENT]...|Region| Numerator | Numerator /      = Leakage  +  Capture + Fission
[PERSENT]...|      |           | Sum[Denominator] |          |           |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|BLAN  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|AXBLK |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|CORE2 | -2.415E+18|        -8.963E-04| 3.564E-05|-3.285E-05| 3.359E-04
[PERSENT]...|CORE1 |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|ROD1  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|ROD2  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|ROD3  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|ROD4  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
[PERSENT]...|ROD5  |  0.000E+00|         0.000E+00| 0.000E+00| 0.000E+00| 0.000E+00
=PERSENT...Parameter General PT of C2_TO_C1P          is -8.96293E-04 denominator
```

Figure 5. Example PERSENT Zone Reactivity Worth/kg Output

In the displayed output, the orientation is setup to be consistent with the user input such that the lower line is the lower edge of the user geometry. The actual values printed in this table of output correspond to the contribution to the perturbation equation from each mesh. A sum of the mesh-wise result will identically produce the parameter value shown at the end of Figure 3.

Similar to the mesh-wise breakdown, the region-wise breakdown is provided where regions are defined by the user in the input and can consist of one or more meshes. The region-wise table can be broken into the individual components of the transport operator as partially shown in Figure 3. If present, area edits, which are collections of regions, can be displayed in a manner similar to the region edits. As was the case with the mesh-wise edits, summation over all regions will produce the parameter value shown at the end of Figure 3.

Another important feature of PERSENT is the ability to represent the reactivity change with respect to the mass change in the domain. Figure 4 shows the calculated mass change in the problem which is a useful check for the user to identify which isotopes are changed and how much change occurs in a particular mesh or region. If the reactivity worth per unit mass is requested, the mass change details are reported first, followed by the reactivity worth, and then the reactivity in worth/kg. Figure 5 shows an output excerpt of the reactivity worth divided by the mesh-wise mass change. It is important to note that if the mass change is zero in the mesh, the reactivity worth is simply zeroed out.

The region-wise output excerpt is used to directly produce input for the SAS4A safety analysis software shown in Figure 1. In addition to the displayed region-wise and mesh-wise results, PERSENT will generate area-wise data consistent with the area definitions in DIF3D which is not included here for brevity. Both the region-wise and area-wise data can be optionally detailed in conventional balance edits, a partial excerpt of which is shown in Figure 5, which are typically used to assess what components of the nuclear data are important in the perturbation. All of these outputs tables must be verified to be accurate as part of the verification work. The input stream and any input options detailed by Figure 2 that can impact these outputs must also be verified to work properly.

In the preceding examples, the exact perturbation (termed generalized perturbation theory in PERSENT as these perturbations are included as components of the sensitivity calculation) details are shown. The first order perturbation details are reported identically to the exact perturbation results as the mathematical details are very similar to the exact perturbation formula [1]. The first order perturbation is a specific approximation of the zone perturbation specified by the user and it must be shown to be accurate and consistent with the desired first order approximation result expected in safety analysis work.

The ADJUST_GENERIC and BOWING_WORTH inputs are newer features of PERSENT. The intention of the ADJUST_GENERIC is to produce spatial distributions of specific radial and axial expansion reactivity coefficients typically used in safety analysis although these have not been adopted at this time. The BOWING_WORTH is a first order based methodology for computing the worth of moving the fuel assemblies to non-centered positions in the hexagonal lattice. It is primarily used to assess the bowing worth in transient analysis to ensure that it provides negative

feedback as desired but has not been adopted as part of the regular safety analysis. The bowing worth needs to be verified as it will likely be used at some level and because adjust_generic is just another way of doing adjust_zone, the additional effort to verify it also is minor.

The other component to consider in perturbation theory is the kinetics parameters. Figure 6 provides example output from PERSENT for the Λ, β, and coalesced kinetics parameters. To calculate the latter two, the user must provide the DLAYXS file which is produced by MC^2 or some equivalent cross section generation code. Because the DLAYXS file does not use self-shielded cross section data, the region-wise cross section definitions do not have to be used and the "SET_DELAY" input option in Figure 2 can be used by the user to link the DLAYXS data to the ISOTXS data. By rule, the PERSENT code will automatically match up the cross section library name included in ISOTXS with that included in DLAYXS such that the user does not have to provide any mapping information (e.g. MC^2 will set the library name for U235 as U235_7 in both ISOTXS and DLAYXS and thus the mapping can easily be identified).

The prompt neutron lifetime, Λ, is directly used in the kinetics equations of SAS4A and other equivalent safety analysis codes that do not use spatial kinetics. Similarly, the effective delayed neutron fraction, β, is typically broken down by delay family, each of which has a decay constant. The coalesced data constitutes a further approximation of the reactor system which is typically valid for short duration transients where the isotopic burnup does not impact the kinetics behavior. While the coalesced formulas were studied in detail in the past, the verification of the PERSENT result should be tested through comparative kinetics solutions of the original system and the coalesced system. As was the case with the regular perturbation options, the mesh-wise and region-wise aspects of Λ and β can be printed and need to be verified. While only Λ and the coalesced β details are typically used, the isotopic breakdown of β will be verified as part of this work. Figure 7 shows the isotopic and group breakdown of the β data that PERSENT will generate if requested. For a significant number of actinides, this output can be very extensive. For β, the verification is relatively straightforward but Λ will be very difficult to verify as it does not have an easy to display calculation methodology.

The sensitivity output is far more extensive than the zone perturbation theory output and Figure 8 through Figure 10 show output excerpts of the sensitivity calculation in PERSENT. Figure 8 shows the output from the sensitivity to an eigenvalue. The purpose of the sensitivity capability is to take the derivative of some design value, termed response, with respect to a cross section. The chosen response is typically something common to reactor analysis projects such as the eigenvalue (criticality), reactivity worth, or the kinetics parameters. In Figure 8, the response is the eigenvalue and the resulting sensitivity vector displays the derivative with respect to each isotope and the cross sections of those isotopes. Figure 9 continues the eigenvalue sensitivity output while Figure 10 shows the output for a reaction rate ratio sensitivity.

For all sensitivity problems, the first section of output from PERSENT is the isotope mapping information as seen in Figure 8. This table of output lists the unique MC^2 based names and how all of the region-wise cross section evaluations provided by the user in ISOTXS map into those names. The PERSENT input allows the user to uniquely map the isotopes as desired. As an example, the PU239H isotope can be treated seperatly from PU239 instead of as part of PU239S.

This isotope mapping is necessary as PERSENT will generate sensitivity vector output with respect to each unique isotope. The rationale behind this approach is that the follow-on UQ calculation has the covariance data arranged by isotope (i.e. U-235, U-238, and Pu-239). Thus there is no point in generating region-wise sensitivity vectors as the UQ perspective will simply merge them together. Because users wanted to investigate the region-wise functionality of the UQ data, Figure 8 and Figure 9 are found to include the zone-wise breakdown of the sensitivity vector followed by the area breaddown of the sensitivity vector and then the whole domain sensitivity vector. The zone-wise sensitivity was chosen as the transport operator naturally decomposes by composition rather than region and that is how the derivative with respect to the cross section data was implemented. By default, all isotopic sensitivities are computed but user input is required to select the isotopes and reactions for which the sensitivity data is printed in the standard output.

```
…
[PERSENT]...Region edits for LAMBDA
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  1.287E+12|         8.570E-10|
[PERSENT]...|BLAN  |  2.366E+13|         1.575E-08|
[PERSENT]...|CORE2 |  1.399E+14|         9.316E-08|
[PERSENT]...|CORE1 |  4.556E+14|         3.034E-07|
[PERSENT]...|ROD1  |  5.826E+12|         3.879E-09|
[PERSENT]...|ROD2  |  2.844E+12|         1.894E-09|
[PERSENT]...|ROD3  |  1.100E+12|         7.323E-10|
[PERSENT]...|ROD4  |  7.423E+12|         4.943E-09|
[PERSENT]...|ROD5  |  2.844E+12|         1.894E-09|
=PERSENT...Parameter LAMBDA Generation time  4.26467E-07 Prompt Lifetime  5.03787E-07 …
[PERSENT]...Region edits for Parameter BETA is
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|BLAN  |  1.021E+17|         6.799E-05|
[PERSENT]...|CORE2 |  1.262E+18|         8.403E-04|
[PERSENT]...|CORE1 |  3.493E+18|         2.326E-03|
[PERSENT]...|ROD1  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD2  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5  |  0.000E+00|         0.000E+00|
=PERSENT...Parameter BETA is         3.23428E-03 denominator  1.50188E+21 k-eff  1.1813033E+00
=PERSENT...Domain coalesced effective point kinetics parameters
=PERSENT...Family     beta(i)    lambda(i)
=PERSENT...   1   1.40541E-03  3.00000E-02
=PERSENT...   2   1.82887E-03  1.00000E+00
…
```

Figure 6. Example PERSENT Output for Λ, β, and the Coalesced Point Kinetics Parameters

```
…
[PERSENT]...Region edits for BETA PU239    family   1
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|REFL  |    1|  0.000E+00|         0.000E+00|
…
[PERSENT]...|CORE2 |    1|  2.711E+17|         1.805E-04|
[PERSENT]...|CORE2 |    2|  1.544E+17|         1.028E-04|
[PERSENT]...|CORE2 |    3|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |-----|  6.080E+18|         4.048E-03|
[PERSENT]...|CORE1 |    1|  6.471E+17|         4.309E-04|
[PERSENT]...|CORE1 |    2|  3.662E+17|         2.438E-04|
[PERSENT]...|CORE1 |    3|  0.000E+00|         0.000E+00|
[PERSENT]...|CORE1 |-----|  1.826E+19|         1.216E-02|
…
[PERSENT]...|Region| Numerator | Numerator /      |
[PERSENT]...|      |           | Sum[Denominator] |
[PERSENT]...|REFL  |  0.000E+00|         0.000E+00|
[PERSENT]...|BLAN  |  0.000E+00|         0.000E+00|
[PERSENT]...|CORE2 |  4.255E+17|         2.833E-04|
[PERSENT]...|CORE1 |  1.013E+18|         6.747E-04|
[PERSENT]...|ROD1  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD2  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD3  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD4  |  0.000E+00|         0.000E+00|
[PERSENT]...|ROD5  |  0.000E+00|         0.000E+00|
=PERSENT...BETA PU239    family   1  9.58046E-04 denominator  1.50188E+21 k-eff  1.1813034E+00
[PERSENT]...Region edits for BETA PU239    family   2
[PERSENT]...|Region|Group| Numerator | Numerator /      |
[PERSENT]...|      |     |           | Sum[Denominator] |
[PERSENT]...|REFL  |    1|  0.000E+00|         0.000E+00|
…
[PERSENT]...|CORE2 |    1|  3.167E+17|         2.109E-04|
[PERSENT]...|CORE2 |    2|  6.764E+16|         4.504E-05|
[PERSENT]...|CORE2 |    3|  0.000E+00|         0.000E+00|
…
=PERSENT...BETA PU239    family   2  8.66242E-04 denominator  1.50188E+21 k-eff  1.1813034E+00
[PERSENT]...Region edits for BETA cumulative PU239
…
```

Figure 7. Example PERSENT Isotopic Breakdown of the β Output

```
…
Index Unique  ISOTXS ->
    1 NA23 5  NA       NAH
    2 FE   5  FE       FEH
    3 O-16 5  O-16
    4 B-10 5  B-10
    5 C    5  C
    6 PU239S  PU239    PU239H
    7 U-238S  U238     U238H
    8 LFPMY2  FP
    9 DUMMY1  DUMP
   10 PU240S  PU240
   11 PU241S  PU241
…
[PERSENT]...Problem REFERENCECORE    is a eigenvalue sensitivity
[PERSENT]...Associated DIF3D output is S_dif3d_problem0001.out
…
[PERSENT]...Sensitivity of the eigenvalue broken down by ZONE
.
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         NA23 5   in zone C1
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -5.924555E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.275864E-04 -1.852417E-05
[PERSENT]...    2            -5.494933E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.537151E-04 -1.537151E-04
[PERSENT]...    3            -4.863934E-04  0.000000E+00  0.000000E+00  0.000000E+00 -5.508319E-04 -5.508319E-04
[PERSENT]...COLUMN SUM       -1.190588E-02  0.000000E+00  0.000000E+00  0.000000E+00 -8.321333E-04 -7.230712E-04
…
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         U-238S   in zone C1
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1             7.201240E-03  3.806282E-02  2.132529E-02  2.132529E-02 -3.817609E-03 -3.817609E-03
[PERSENT]...    2            -2.584789E-02  1.241734E-04  7.204143E-05  7.204143E-05 -2.139410E-02 -2.139410E-02
[PERSENT]...    3            -6.588721E-02  3.473586E-05  2.216898E-05  2.216898E-05 -6.597191E-02 -6.597191E-02
[PERSENT]...COLUMN SUM       -8.453386E-02  3.822173E-02  2.141950E-02  2.141950E-02 -9.118362E-02 -9.118362E-02
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         NA23 5   in zone C2
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -5.633778E-03  0.000000E+00  0.000000E+00  0.000000E+00 -2.168730E-04 -3.148763E-05
[PERSENT]...    2            -6.293962E-04  0.000000E+00  0.000000E+00  0.000000E+00 -2.345501E-04 -2.345501E-04
[PERSENT]...    3             2.243098E-03  0.000000E+00  0.000000E+00  0.000000E+00 -8.075592E-04 -8.075592E-04
[PERSENT]...COLUMN SUM       -4.020077E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.258982E-03 -1.073597E-03
…
```

Figure 8. Example PERSENT Sensitivity Output Broken Down by Zone

```
…
[PERSENT]...Sensitivity of the eigenvalue broken down by AREA
.
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         NA23 5   and area   TCORE
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -1.155833E-02  0.000000E+00  0.000000E+00  0.000000E+00 -3.444593E-04 -5.001180E-05
[PERSENT]...    2            -6.124329E-03  0.000000E+00  0.000000E+00  0.000000E+00 -3.882651E-04 -3.882651E-04
[PERSENT]...    3             1.756705E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.358391E-03 -1.358391E-03
[PERSENT]...COLUMN SUM       -1.592596E-02  0.000000E+00  0.000000E+00  0.000000E+00 -2.091116E-03 -1.796668E-03
…
[PERSENT]...Sensitivity of the eigenvalue over the whole domain
.
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         NA23 5
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -1.323321E-02  0.000000E+00  0.000000E+00  0.000000E+00 -4.289948E-04 -6.228544E-05
[PERSENT]...    2            -5.900067E-03  0.000000E+00  0.000000E+00  0.000000E+00 -4.969010E-04 -4.969010E-04
[PERSENT]...    3             3.399640E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.767197E-03 -1.767197E-03
[PERSENT]...COLUMN SUM       -1.573363E-02  0.000000E+00  0.000000E+00  0.000000E+00 -2.693093E-03 -2.326384E-03
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         FE   5
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -1.662329E-02  0.000000E+00  0.000000E+00  0.000000E+00 -2.831488E-03 -1.017995E-03
[PERSENT]...    2            -7.701737E-03  0.000000E+00  0.000000E+00  0.000000E+00 -9.002929E-03 -9.002388E-03
[PERSENT]...    3            -4.905355E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.298344E-02 -1.298344E-02
[PERSENT]...COLUMN SUM       -2.923038E-02  0.000000E+00  0.000000E+00  0.000000E+00 -2.481786E-02 -2.300382E-02
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         O-16 5
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -1.493182E-02  0.000000E+00  0.000000E+00  0.000000E+00 -2.110756E-03 -7.252783E-09
[PERSENT]...    2            -1.374828E-02  0.000000E+00  0.000000E+00  0.000000E+00 -5.675265E-08 -5.675265E-08
[PERSENT]...    3             5.567436E-03  0.000000E+00  0.000000E+00  0.000000E+00 -1.967746E-07 -1.967746E-07
[PERSENT]...COLUMN SUM       -2.311266E-02  0.000000E+00  0.000000E+00  0.000000E+00 -2.111009E-03 -2.607801E-07
[PERSENT]...Sensitivity of the eigenvalue      1.173141 to isotope:         B-10 5
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1             0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
[PERSENT]...    2             0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
[PERSENT]...    3             0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
[PERSENT]...COLUMN SUM        0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
…
```

Figure 9. Example PERSENT Sensitivity Output Broken Down by Area and Total

```
…
[PERSENT].....................................................................................
[PERSENT]...Problem RATIO_P39F_U38C  is a reaction rate ratio sensitivity
[PERSENT]...Associated DIF3D output is S_dif3d_problem0005.out
[PERSENT].....................................................................................
[PERSENT]...Calling the inhomogeneous fixed source driver for the adjoint Gamma
[PERSENT]...|Iter|Outers|Total |pM| Full Error | Target |Flat P0 Err |   Target   | FM removal  initial |
%PERSENT]...|   1|     5|     5|Y | 1.5969E+00 > 1.0E-3 | 1.7321E+00 >  1.0000E-05| 2  1.8E-17  3.5E-02 |
%PERSENT]...|   2|     5|    10|Y | 1.2665E+02 > 1.0E-3 | 2.0434E+00 >  1.0000E-05| 2  9.0E-18  3.8E-03 |
%PERSENT]...|   3|     5|    15|Y | 2.9523E+00 > 1.0E-3 | 3.4051E-04 >  1.0000E-05| 2  9.0E-18  4.6E-03 |
%PERSENT]...|   4|     5|    20|Y | 5.1611E-01 > 1.0E-3 | 1.1541E-04 >  1.0000E-05| 2  3.3E-17  4.6E-03 |
%PERSENT]...|   5|     5|    25|Y | 2.7669E-01 > 1.0E-3 | 2.7339E-05 >  1.0000E-05| 2  1.4E-17  4.9E-03 |
%PERSENT]...|   6|     5|    30|Y | 1.1880E-01 > 1.0E-3 | 6.4508E-06 <  1.0000E-05| 2  5.5E-18  4.8E-03 |
%PERSENT]...|   7|     5|    35|N | 1.0193E+00 > 1.0E-3 | 1.9684E-02 >  1.0000E-05| 2  2.2E-17  2.2E-02 |
%PERSENT]...|   8|     5|    40|N | 1.5028E+00 > 1.0E-3 | 4.0984E-02 >  1.0000E-05| 2  9.4E-18  2.3E-02 |
%PERSENT]...|   9|     5|    45|N | 3.4681E+00 > 1.0E-3 | 1.6706E-01 >  1.0000E-05| 2  5.3E-18  4.3E-03 |
%PERSENT]...|  10|     2|    38|N | 1.6717E+00 > 1.0E-3 | 3.4641E-01 >  1.0000E-05| 2  1.6E-16  8.7E-02 |
%PERSENT]...|  11|     2|    40|N | 8.2882E-01 > 1.0E-3 | 8.4368E-02 >  1.0000E-05| 2  4.8E-17  3.3E-02 |
%PERSENT]...|  12|     2|    42|N | 1.0445E+00 > 1.0E-3 | 4.1834E-02 >  1.0000E-05| 2  4.1E-17  1.6E+00 |
%PERSENT]...|  13|     1|    43|N | 6.3363E+02 > 1.0E-3 | 1.5582E+00 >  1.0000E-05| 2  9.6E-18  3.3E-03 |
%PERSENT]...|  14|     1|    44|N | 3.9665E+00 > 1.0E-3 | 2.5948E+00 >  1.0000E-05| 2  1.9E-17  3.9E-02 |
%PERSENT]...|  15|     1|    45|N | 1.8341E+00 > 1.0E-3 | 5.2220E-01 >  1.0000E-05| 2  4.7E-18  9.8E-03 |
%PERSENT]...|  16|     1|    46|N | 1.3322E+00 > 1.0E-3 | 3.7026E-01 >  1.0000E-05| 2  1.3E-17  2.1E-02 |
%PERSENT]...|  17|     1|    47|N | 1.5385E+00 > 1.0E-3 | 3.1031E-02 >  1.0000E-05| 2  5.9E-17  4.9E-03 |
%PERSENT]...|  18|     1|    48|N | 5.3628E-01 > 1.0E-3 | 9.8973E-02 >  1.0000E-05| 2  3.9E-17  4.0E-03 |
%PERSENT]...|  19|     1|    49|N | 3.5058E-01 > 1.0E-3 | 3.8231E-01 >  1.0000E-05| 2  1.3E-20  7.1E-03 |
%PERSENT]...|  20|     1|    50|N | 2.1409E-01 > 1.0E-3 | 9.5310E-02 >  1.0000E-05| 2  1.0E-17  9.7E-03 |
…
%PERSENT]...|  29|     2|   103|N | 8.5052E-04 > 1.0E-3 | 1.0651E-05 >  1.0000E-05| 2  2.8E-17  1.6E-03 |
%PERSENT]...|  30|     2|   105|N | 2.5654E-04 < 1.0E-3 | 3.8180E-06 <  1.0000E-05| 2  2.4E-17  1.6E-03 |
[PERSENT]...Sensitivity of the    FISSION /CAPTURE   macro reaction rate ratio      1.747982 to isotope:      U-238S
=PERSENT]...or sensitivity of the FISSION /CAPTURE   micro reaction rate ratio      6.292736 to isotope:      U-238S
[PERSENT]...GROUP   ALPHA->    TOTAL         NU            NUFISSION     FISSION       CAPTURE       GAMMA
[PERSENT]...    1            -6.805380E-02 -2.392720E-03 -2.861094E-03 -2.861094E-03 -3.700099E-02 -3.700099E-02
[PERSENT]...    2            -2.401029E-01 -1.327885E-05  1.088247E-05  1.088247E-05 -2.057973E-01 -2.057973E-01
[PERSENT]...    3            -6.263114E-01 -5.214840E-06  1.915259E-05  1.915259E-05 -6.194722E-01 -6.194722E-01
[PERSENT]...COLUMN SUM       -9.344681E-01 -2.411214E-03 -2.831059E-03 -2.831059E-03 -8.622705E-01 -8.622705E-01
…
```

Figure 10. Example PERSENT Reaction Rate Ratio Sensitivity Output

In Figure 8 through Figure 10 the sensitivity vector details are found to be listed for each unique isotope and broken into group and reaction rate components. This breakdown is again motivated by the needs in the UQ calculation. It is important to note that PERSENT will generate sensitivities for reaction rates that are not needed in a conventional UQ calculation (such as TOTAL in Figure 8). Because of this, not all of the reactions will be verified which is left for discussion in the verification report.

As discussed, the sensitivity coefficients of interest include β, Λ, k_{eff}, reactivity worth, and reaction rate ratio. The k_{eff} and reactivity worth approach to computing the sensitivity vector only require the forward and adjoint flux solutions for the base and perturbed reactor models. For β, Λ, and the reaction rate ratio the simple derivative of the transport equation with respect to the cross section requires additional coupling information, termed Γ, to be computed which is obtained via the solution of a special inhomogeneous fixed source problem. For β and Λ, an adjoint and forward Γ must be solved while for the reaction rate ratio sensitivities, only an adjoint Γ is needed.

DIF3D presently includes an inhomogeneous fixed source calculation capability which is described elsewhere [3] and was verified as part of the DIF3D verification work [20]. The typical constraint for this solver to work is that the associated eigenvalue problem (for fission source driven problems) is sub-critical. There is no steady state flux solution for the problem if the eigenvalue problem is critical or super-critical. For the sensitivity formalism, the base state provided by the user is normally slightly super-critical and thus the built in inhomogeneous fixed source solution algorithm cannot produce a solution. This would seem to be at odds with the capabilities of DIF3D, but the reason the Γ sensitivity problem is tractable is because the fixed source and Γ solution are defined to be orthogonal to the fundamental mode solution. In this circumstance, there is a solution to the steady state problem being proposed regardless of the criticality state. To modify the solver capability directly in DIF3D required significant structural changes to DIF3D which were not achievable due to the costs associated with updating all of the interconnected parts of the ARC system.

The approach taken in PERSENT was to solve the Γ problems by using multiple DIF3D restart calculations. For DIF3D-FD, this would be a minor additional computational cost but for DIF3D-VARIANT it is a very expensive process as the response matrices have to be computed multiple times and the NHFLUX files pose substantial I/O requirements. In DIF3D, a steady state problem with a fixed source will typically see rapid convergence of the flux solution and require 2 or 3 outer iterations worth of computational effort. Ignoring acceleration of the power method, for a steady state eigenvalue problem with a low dominance ratio, the convergence of the eigenvalue system in DIF3D will typically take less than 30 outer iterations. Conversely, an eigenvalue problem with a dominance ratio of 0.99999 can take thousands of iterations. Similarly, a conventional inhomogeneous problem with a sub-critical eigenvalue and high dominance ratio can take thousands of outer iterations to converge in DIF3D. Conventional acceleration methodologies implemented for the eigenvalue problem do not apply to the Γ inhomogeneous eigenvalue problem because of the orthogonality and thus the functional solver strategy of PERSENT can pose extreme computational costs without even considering the costs associated with the restart process itself.

As inferred, because the Γ problem can involve a significantly supercritical model, the Γ flux solution can grow rapidly if it is not orthogonal to the fundamental mode. The constraint that the Γ solution be orthogonal requires an orthogonalization process, termed fundamental mode contamination removal, which should be performed as frequently as possible. The orthogonalization process is preformed and monitored by PERSENT and the number of outer iterations performed by DIF3D in each restart is adjusted appropriately.

What is shown at the top of Figure 10 is the control process inside of PERSENT for the inhomogeneous solver. Each line that starts with a % indicates the outcome of a restart call to DIF3D. The output is listed with respect to the number of restart calls (Iter) where each line lists the number of outers performed by DIF3D and the cumulative number of outers used to solve the problem along with a flag indicating whether the partitioned matrix acceleration strategy was used. Note that the partitioned matrix acceleration strategy is focused on converging the fundamental mode solution and thus can rapidly lead to fundamental mode contamination. The next four columns in Figure 10 show the iterative error on the full flux vector (full error) and the isotropic diffusion component (Flat P0 Err) along with the error targets. These iterative flux errors correspond to the relative difference between the solution vector provided as the guess to DIF3D and the one returned from DIF3D after the fundamental mode contamination has been removed.

The last three columns of the top table in Figure 10 can be used to indicate how much the fundamental mode has perturbed the solution being returned by DIF3D. The first number indicates how many fundamental mode (FM) orthogonalization steps were required to achieve the error on the orthogonalization norm. More than 2 iterations indicates severe drift in the overall solution and PERSENT will act quickly to constrict the outer iteration limit. The last column indicates the magnitude of the fundamental mode contamination in the Γ solution returned from DIF3D. As can be seen, the fundamental mode contamination was as up to 160% and as low as 0.2%. In this example output, it should be clear that the fundamental mode contamination is very severe (strong super-criticality) as PERSENT adjusts the number of outers to 1 and disables the partitioned matrix acceleration. The outer iteration limit can be provided by the user such that the computational effort invoked in the first 9 restart calculations could be avoided. Only after adjusting the number of outers to 1 does the iterative flux errors start to decrease and achieve convergence.

For the verification work, the functional use of the PERSENT solver will require testing on a sub-critical, critical, and super-critical reactor model. High dominance ratio problems do not specifically need to be tested as they should simply be more computationally expensive versions of the other cases. While it is relatively easy to verify that the Γ solution and its fixed source are orthogonal to the fundamental mode flux solution, it is a non-trivial exercise to verify that the fixed source and obtained Γ solution are mathematically correct for a given problem. Further, it is very difficult to verify that the applied functional is generating the correct sensitivity vector internal to PERSENT given the Γ solution. Thus, for verification of the sensitivity vectors, the classic finite difference approach to evaluating the cross section sensitivities will be utilized. For a 33 group cross section set with 100 unique isotopes, and 6 reactions (nu, fission, capture, elastic scattering, inelastic scattering, chi), this is equivalent to running 19800 DIF3D calculations. While restart calculations can be used to reduce the true burden, the reality is that the finite difference

methodology needs significantly more work because each cross section has to be perturbed enough to see the impact on the response (eigenvalue, reaction rate ratio, Λ, etc…) in the output which is not easy to know ahead of time. It is important to note that the eigenvalue and flux error convergence for DIF3D are normally reduced substantially in order to eliminate iterative error noise in the computed sensitivity vector when applying the finite difference technique. In total, using the finite difference methodology on a real reactor problem is computationally intractable and a more simplified test case will be used for the verification work.

The sensitivity vector output for the reaction rate ratio output in Figure 10 is presented identically to the eigenvalue sensitivity results of Figure 9. The only exception is an additional line for the reaction rate ratio to indicate the nominal reaction that the sensitivity vector is being generated for (i.e. the fission/capture micro reaction rate ratio of 6.292736 is reported). From this section, it should come as no surprise that verification of the sensitivity capability is going to take a considerably larger amount of effort than that of the perturbation theory verification.

The last capability that is featured in PERSENT is the ability to apply the uncertainty quantification (UQ) and representativity operations. Figure 11 and Figure 12 show example output excerpts from PERSENT for the UQ operation. The representativity relationship is defined as

$$R = \frac{s_1^T \cdot D \cdot s_2}{\sqrt{s_1^T \cdot D \cdot s_1} \cdot \sqrt{s_2^T \cdot D \cdot s_2}}, \quad (1)$$

where s_1 is the sensitivity vector from one model and s_2 is the sensitivity vector from another reactor model and the matrix D is the covariance matrix. Treating them in conventional matrix-vector notation requires application of the transpose of s_1 in equation 1. For UQ calculations the formula is simply

$$UQ = \sqrt{s_1^T \cdot D \cdot s_1}, \quad (2)$$

and thus one can see how the two operations are related. Internal to PERSENT, all of these operations are termed UQ operations even though the calculation itself can be part of the representativity numerator or denominator work. By design, the intention of the representativity approach is to combine the sensitivity vector from two reactor models together such as projecting a reaction rate measurement in ZPPR onto the target reactor being designed as an example. PERSENT cannot presently handle more than a single ISOTXS file and merging the ISOTXS data from two different models is considerably impractical. Thus the design of the PERSENT software is to store the sensitivity vector from a given model to be used in a later PERSENT calculation of UQ or representativity. Thus verification work not only has to focus on the UQ calculation, but also the sensitivity vector storage feature as these are critical components of the validation work.

Starting with the output excerpt in Figure 11, the output is the important part of the UQ routine. The first line indicates the file that the user provided covariance matrix was imported from where the covariance matrix is discussed in the literature [21]. The covariance matrix is a fixed format similar to ISOTXS but its contents can vary considerably with respect to the connections between reactions of the various isotopes depending upon the evaluator. To date, users have only tried one covariance matrix and the verification work needs to test the full capabilities of the covariance matrix to ensure it is working properly.

The next line of importance for UQ is the WARNING statement that indicates only 70 lines of the 416 available were used where a "line" is a block of data that connects a reaction of a given isotope to a reaction of another isotope (or itself). The number 416 indicates that there are 416 reaction/isotope connections in the data file that can be used in the UQ calculation to form the D matrix above. The warning message thus indicates that only 70 of the available lines were used in constructing the D matrix. Because the UQ data file, COMMARA in this case, is generated external to MC^2, the user must map the isotope and reaction names in their data file with COMMARA_ISOTOPE and COMMARA_REACTION shown earlier in Figure 2.

The unique isotope identification list used by the UQ routine is identical to that used in building the sensitivity vector. Internal to PERSENT, the covariance matrix is built to only consider those isotopes and reactions identified in the model and the unused data is discarded. In this example problem, only a small set of isotopes were included and thus most of the covariance information is not used. This output is particularly important as it informs the user to check their mapping relationships to ensure that isotopic data is not ignored. In the later sections of output, a missing isotope mapping will result in no covariance data and thus the isotope contribution to the UQ problem being solved will be zero even if it is not supposed to be zero.

The remaining UQ output structure is a series of different ways of displaying the contribution to uncertainty. Each section of this output is optional except for the final line which displays the total UQ result. In Figure 11, the first table of output is the isotope/reaction to isotope/reaction. In this case, the matrix relationships in equation 1 and 2 are reported individually by isotope/reaction. The mathematics are described in the PERSENT manual [1] and the breakdown yields imaginary numbers as the partial results can be negative values. Row sum and column sum values are provided for each table of isotope data. It is important to point out that the reaction list is truncated for each isotope according to the reactions present in the covariance matrix and it is provided in a set of principle reactions followed by scattering reactions. As an example, the oxygen isotope only has capture, elastic, and inelastic scattering reactions. The output for n-2n and n-alpha reactions is not generated by PERSENT in either table even though they are possible from the covariance matrix definition. The provided U-238 result shows how the principle reaction list is expanded when other reactions are present. As discussed previously, for those unique isotopes with no covariance data or missing mapping to covariance data, there will be no output printed in this section.

The next table of output is seen in Figure 12 termed isotope to isotope. This table is not typical of UQ or representativity operations but it can readily show the interplay between isotopes when provided in covariance matrix. It is truncated to only consider those isotopes which are present in the reactor model. The last table of output is the summary table by isotope and reaction [1]. This table is much more relevant to UQ work as it indicates which reactions of which isotopes dominate the total uncertainty. It should be clear from the output table that many isotopes were either not present in the reactor model (i.e. U-234) or the covariance mapping data was not provided leading to a zero contribution. Combined, the UQ output provides the user with valuable details on the isotopic breakdown of the final UQ product and thus all of the tables of output need to be verified as part of the verification work.

```
…
[COMMARA]...Importing data from bnl.1.apr.2011.commara.with.chi.mubar.matrix
[PERSENT]...Checking the PERSENT input data for the perturbation options
[PERSENT]...Checking the PERSENT input data for the sensitivity options
[PERSENT]...WARNING::: Only using     70 of the available    416 COMMARA matrix lines?
…
[PERSENT].....................................................................................................
[PERSENT]...                      Performing a Uncertainty Quantification Assessment on Problem: REFERENCECORE
[PERSENT].....................................................................................................
[PERSENT]...               Detailed Table of Data for Isotope/Reaction from Isotope/Reaction to Follow
[PERSENT].....................................................................................................
[PERSENT]...    Summary of uncertainty computation for isotope O16__7   reaction CAPTURE
[PERSENT]...             O16__7
[PERSENT]...Group       CAPTURE          Column Sum
[PERSENT]...    1     3.997025E-04     3.997025E-04
[PERSENT]...    2     1.002654E-03     1.002654E-03
[PERSENT]...    3     1.301398E-03     1.301398E-03
[PERSENT]...    4     1.435073E-04     1.435073E-04
[PERSENT]...    5     1.506607E-06     1.506607E-06
…
[PERSENT]...    Summary of uncertainty computation for isotope O16__7   reaction ELASTIC
[PERSENT]...             O16__7           O16__7
[PERSENT]...Group       ELASTIC          INELASTIC        Column Sum
[PERSENT]...    1     7.707611E-07     2.179046E-06*i   2.038178E-06*i
[PERSENT]...    2     4.367374E-06     1.143952E-05*i   1.057302E-05*i
[PERSENT]...    3     1.836868E-05     0.000000E+00     1.836868E-05
[PERSENT]...    4     5.316071E-05*i   0.000000E+00     5.316071E-05*i
…
[PERSENT]...    Summary of uncertainty computation for isotope U238_7   reaction ELASTIC
[PERSENT]...             U238_7           U238_7           U238_7           U238_7           U238_7
[PERSENT]...Group       FISSION          CAPTURE          ELASTIC          INELASTIC        N2N              Column Sum
[PERSENT]...    1     3.873128E-06*i   0.000000E+00     1.576015E-05     3.765818E-05     5.595910E-06     4.102236E-05
[PERSENT]...    2     1.233242E-05*i   0.000000E+00     1.633237E-04     5.003341E-04     5.841782E-05     5.294047E-04
[PERSENT]...    3     0.000000E+00     0.000000E+00     4.715112E-04     1.473609E-03     0.000000E+00     1.547206E-03
…
```

Figure 11. Example PERSENT Covariance Matrix Calculation Output Part 1

```
…
[PERSENT].....................................................................................................
[PERSENT]...                          Summary Table of Data for Isotope from Isotope to Follow
[PERSENT].....................................................................................................
[PERSENT]...Summary of overall uncertainty data by isotope
[PERSENT]...Isotope          O16__7          U238_7          PU2397          PU2407          PU2417          FE56_7
[PERSENT]...O16__7     1.766917E-03     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00   0.000000E+00
[PERSENT]...U238_7     0.000000E+00     1.283190E-02     0.000000E+00     0.000000E+00     0.000000E+00   0.000000E+00
[PERSENT]...PU2397     0.000000E+00     0.000000E+00     3.905468E-03     0.000000E+00     0.000000E+00   0.000000E+00
[PERSENT]...PU2407     0.000000E+00     0.000000E+00     0.000000E+00     3.122052E-03     0.000000E+00   0.000000E+00
[PERSENT]...PU2417     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     7.575845E-04   0.000000E+00
[PERSENT]...FE56_7     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00   6.895036E-03
[PERSENT]...NA23_7     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00   0.000000E+00
[PERSENT]...U235B      0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00   0.000000E+00
[PERSENT]...U235D      0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00   0.000000E+00
[PERSENT]...Total      1.766917E-03     1.283190E-02     3.905468E-03     3.122052E-03     7.575845E-04   6.895036E-03
…
[PERSENT].....................................................................................................
[PERSENT]...                      Summary Table of Uncertainty Quantification Calculation to Follow
[PERSENT].....................................................................................................
[PERSENT]...    Summary of overall uncertainty data by reaction
[PERSENT]...    Isotope                   NU          FISSION          CAPTURE           GAMMA            ALPHA
[PERSENT]...        O16__7       0.000000E+00     0.000000E+00     1.696857E-03     0.000000E+00     0.000000E+00
[PERSENT]...        MO92_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        MO94_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        MO95_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        MO96_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        MO97_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        MO98_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        MO1007       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        U234_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        U235_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        U236_7       0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00     0.000000E+00
[PERSENT]...        U238_7       1.801342E-03     5.043630E-04     3.065919E-03     0.000000E+00     0.000000E+00
…
=PERSENT]...Total UQ product for problem REFERENCECORE              S*C*S =  2.451178E-04 square root =  1.565624E-02
```

Figure 12. Example PERSENT Covariance Matrix Calculation Output Part 2

2.2 PERSENT Identified Verification Tasks

The preceding dissection and identification of the output used in commercial reactor projects, yields a set of tasks to accomplish as part of the verification work. Table 1 gives the identified task list for the verification work where the category number refers to a specific functional use for the PERSENT software.

Most reactor projects exclusively use either the hexagonal or triangular-Z geometry options of DIF3D and thus those are the primary focus of the PERSENT verification work. However, because PERSENT only deals with DIF3D-VARIANT, only the hexagonal geometry option is really applicable. Since ZPPR data is used as part of the validation work, Cartesian geometry options will also have to be verified as the sensitivity calculations will be performed using ZPPR problems. Since the operator between these two geometries is different and both are coded up internally to PERSENT, both options will need to be checked in each category. In Table 1, the work has been organized into six categories according to the type of work and checking that needs to be done. The action of completing each category will cover the verification of all of the preceding output examples.

In the first category, the focus is placed on the proper execution of the DIF3D software. This step is important as it verifies that the entire perturbation or sensitivity calculation is actually consistent with the desired problem. In the second category, the exact perturbation theory function of PERSENT is tested focusing on the zone perturbation option. Category 3 is focused on the first order perturbation capability and has many of the same requirements as category 2. The main exception is to demonstrate that the first order perturbation theory approach is infact a first order approximation of the exact perturbation result. Category 4 is focused on the kinetics parameters which involves no physical perturbation to the problem but simply verification that the quantities are calculated correctly. Category 5 is focused on the accuracy of the sensitivity vectors and is likely the most time consuming aspect because of all of the finite difference calculations that will be needed. This category also verifies the unique isotope mapping is functioning properly, being obeyed, and that the import and export of sensitivity vectors is working. Category 6 is focused on verification of the UQ calculation details.

In practice, the companion verification document will work through each verification test problem that is created and selectively demonstrate how the above tasks are satisified by the verification problem and which output tables are being verified.

Table 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

3 Planned Verification Exercises

This section will summarize the anticipated test problems and how they will satisfy the verification tasks in each of the six categories identified in Table 1.

3.1 Verification Methodology for the Perturbation Capability

Analytic solutions of the exact perturbation and sensitivity vectors are relatively difficult and limited to problems for which analytic solutions to the diffusion or transport equation are possible. As these problems would not be very complex, the PERSENT work will not focus on using analytic based benchmark solutions. Instead, it will rely upon the DIF3D verification work and assume that the solution provided by DIF3D-VARIANT is accurate with respect to the matrix-vector system. The verification that the execution of DIF3D from PERSENT is consistent with the regular DIF3D process is thus key to the verification effort.

Another aspect of PERSENT that will be used in the verification process is the ability to import a flux vector obtained with DIF3D. That pathway can be abused to allow the various components of the perturbation to be trivially computed. To explain, the transport operator can be artificially collapsed to a crude neutron balance on each mesh by providing PERSENT with a P_0 flat flux solution in each mesh. This allows the entire perturbation calculation to be carried out by hand, or within EXCEL for large data sets, without the need to program the entire transport operator. This can be done regardless of the actual flux solution to a given problem. This technique can be used for both the exact and first order perturbation functions and the flux vector itself can be verified to be setup properly using the utility program EvaluateFlux. This approach, along with standard direct DIF3D calculations of the spatial reactivity worth, will be used to evaluate category 2 and 3.

3.2 Verification Methodology for the Kinetics Parameters

The kinetics parameter for Λ is particularly painful to verify. The same P_0 flat flux technique described above will need to be used as there is no other option to check the validity of the PERSENT result except a hand calculation of a simple problem or results from another perturbation theory code. Unlike Λ, the β and its component parts can be calculated by manipulation of the input data. To explain, when targeting a single delay family of a given isotope, the remaining kinetics data for all isotopes and delay families can be set to zero and the regular PERSENT calculation will simply display the component piece that was not deleted. The P_0 flat flux technique can also be used to verify the components of β. The coalesced kinetics parameter feature will be tested by building a simple point kinetics code (or using one that already exists) that demonstrates the kinetics response of the coalesced system is consistent with the originating system. Because the isotopic detail is lost in a coalesced system, the primary focus would be to ensure the response of power is correct in the kinetics calculations.

3.3 Verification Methodology for the Sensitivity Vector

The sensitivity vector is by far the most difficult aspect to verify in PERSENT. The most reliable means of verifying the eigenvalue sensitivity is to use the finite difference methodology. In this methodology, the cross section data for a reaction of each isotope is perturbed individually and a new DIF3D calculation is obtained. The change in cross section and change in eigenvalue are merged to define a linear coefficient for the perturbation. This process can be very expensive as it can involve thousands of DIF3D calculations but it will be required to verify the sensitivity vector

details. Effort to minimize the computational work required to verify the sensitivity vector will be key to this verification task.

In addition to the finite difference methodology, the P_0 flat flux technique can also be used to allow the sensitivity vector components of the eigenvalue problem to be hand calculated. This approach can be made to work with all of the sensitivity options as the Γ solutions can also be provided as P_0 flat distributions. A series of verification test problems will have to be constructed where the finite difference or hand calculated results provide the reference solution. Beyond the eigenvalue and reactivity worth sensitivity vectors, the remaining sensitivity vectors will require finite difference calculations through PERSENT (Λ and β in particular) as those capabilities are not normally part of the DIF3D output.

3.4 Verification Methodology of the UQ Capability

The first test of the UQ capability would be to create a fictitious covariance matrix and ensure that it is loaded and applied correctly. Because the sensitivity vector can consist of thousands of moments (isotopes, reactions, energy groups) for even simple problems, this will require some kind of verified external calculation capability of the matrix-vector product. A more practical option would be to fabricate the sensitivity vector along with the covariance data such that the matrix vector product yields a simple result. The three tables that break down the contribution would also be able to be checked by manipulation of the incoming sensitivity vector. In this manner, the entire UQ capability can be checked independent of the actual problem being provided to PERSENT.

4 Conclusion

This manuscript described the PERSENT capabilities that are used as part of commercial reactor projects. In that process, the PERSENT capabilities required to support reactor design projects were displayed and discussed. These requirements were then extended into the verification tasks and a set of identified test cases which can be used to perform the actual verification. This verification work is planned to be performed using the latest version of PERSENT. Further, the verification work will be automated as much as practical so it can be trivially repeated for future PERSENT releases and operating environments.

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