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*Verification of the MCNP™  
Perturbation Correction Feature  
for Cross-Section Dependent Tallies*

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for Cross-Section Dependent Tallies*

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# TABLE OF CONTENTS

ABSTRACT.....	1
I. INTRODUCTION .....	2
II. THEORY .....	3
A. Derivation of the Operator.....	3
1. First Order.....	6
2. Second Order .....	10
B. Implementation in MCNP .....	14
III. USER INTERFACE.....	15
A. PERT Card .....	15
1. General Description .....	15
2. PERT Card Keywords .....	16
B. FM Card.....	18
1. Description of the FM Card .....	18
2. Reaction Numbers.....	19
C. Perturbation Correction Capability for Cross-Section Dependent Tallies .....	20
D. Perturbation and Correction Cautions.....	21
IV. CAPABILITY VERIFICATION.....	22
A. Validation of MT Versus FM Reaction Numbers .....	22
B. Neutron and Photon Perturbation with Specified RXN.....	23
C. Lists of RXN Numbers .....	23
D. Nonsequentially Numbered Cells .....	24
E. Positive and Negative RHO Numbers .....	25
F. Bogus RXN, CELL, MAT, and METHOD Numbers .....	26
1. Neutron Problem with Photon Reaction on RXN Parameter .....	26
2. Unknown Reaction on RXN Parameter.....	26
3. Use of Nonexisting Cell on CELL Parameter .....	27
4. Use of Nonexisting Material on MAT Parameter.....	27
5. Use of Invalid Number on METHOD Parameter .....	27
6. Bogus Parameter Findings .....	27
G. Energy Ranges Via the ERG Parameter.....	28
H. Effect on Other Tally Types .....	29
V. FURTHER CROSS-SECTION-DEPENDENT TALLY VERIFICATION TESTS .....	31
A. Godiva–Density Perturbation .....	31
B. Godiva–Composition Change.....	33
C. Test Problem INP18– $K_{\text{eff}}$ Estimate .....	33
D. Test Problem INP02–Neutron Absorption Rate Estimate .....	35
E. Test Problem INP04–Photon Collision Rate Estimate.....	37
F. Test Problem INP10–Photon Collision Rate Estimate.....	39

VI. PERTURBATION CONVERGENCE .....	41
A. Neutron Density Perturbation Problem.....	41
B. Neutron Material Perturbation Problem .....	42
C. Photon Density Perturbation Problem with Nonsequentially Numbered Cells .....	42
D. Neutron KCODE Density and Repeated Nuclide Perturbation Problem .....	43
VII. UPGRADE OF INSTALLATION TEST SUITE .....	44
A. Changes to Suite Problem Inp10 .....	45
B. Changes to Suite Problem Inp11.....	45
C. Changes to Suite Problem Inp18 .....	45
VIII. SUMMARY .....	46
REFERENCES .....	46
APPENDIX A.....	47
I. OVERVIEW .....	47
II. TEST INPUT FILES .....	47
A. Validation of MT Versus FM Reaction Numbers .....	47
1. Input File Mtfm01.....	47
2. Input File Mtfm02.....	48
3. Input File Mtfm03.....	48
4. Input File Mtfm06.....	48
5. Input File Mtfm31.....	49
6. Input File Mtfm32.....	49
7. Input File Mtfm33.....	49
8. Input File Mtfm34.....	50
9. Input File Mtfm35.....	50
10. Input File Mtfm81.....	50
11. Input File Mtfm82.....	51
12. Input File Mtfm83.....	51
B. Reaction List on RXN Parameter .....	51
1. Input File Lis01.....	52
2. Input File Lis31.....	52
C. Nonsequentially Numbered Cells .....	53
1. Input File Mis01.....	53
2. Input File Mis01b.....	54
3. Input File Mis31.....	54
4. Input File Mis31b.....	55
D. Positive and Negative RHO Numbers .....	56
E. Bogus RXN, CELL, MAT, and METHOD Numbers .....	56
1. Neutron Problem with Photon Reaction on RXN Parameter .....	56
2. Unknown Reaction on RXN Parameter.....	57
3. Use of Nonexisting Cell on CELL Parameter .....	57
4. Use of Nonexisting Material on MAT Parameter.....	57
5. Use of Invalid Number on METHOD Parameter .....	57

F. Energy Ranges Via the ERG Parameter.....	57
1. Input File Erg01 .....	57
2. Input File Erg02 .....	58
3. Input File Erg03 .....	58
G. Effect on Tally Types 6 and 7 .....	59
1. Input File Tal61 .....	59
2. Input File Tal61b .....	60
3. Input File Tal62 .....	60
4. Input File Tal62b .....	60
5. Input File Tal63 .....	61
6. Input File Tal63b .....	61
7. Input File Tal71 .....	61
8. Input File Tal71b .....	62
H. Perturbation Convergence.....	62
1. Input File Fm71 .....	62
2. Input File Fm71b .....	63
3. Input File Fm72 .....	63
4. Input File Fm72b .....	64
5. Input File Fm73 .....	64
6. Input File Fm73b .....	64
7. Input File Fm75 .....	65
8. Input File Fm75b .....	65
APPENDIX B .....	67
I. GODIVA-DENSITY PERTURBATION.....	67
II. GODIVA-COMPOSITION CHANGE .....	68
III. TEST PROBLEM INP18- $K_{\text{eff}}$ ESTIMATE.....	69
IV. TEST PROBLEM INP02-NEUTRON ABSORPTION RATE ESTIMATE .....	72
V. TEST PROBLEM INP04-PHOTON COLLISION RATE ESTIMATE .....	74
VI. TEST PROBLEM INP10-PHOTON COLLISION RATE ESTIMATE .....	76
APPENDIX C .....	79
I. OVERVIEW .....	79
A. Voiding and Unvoiding .....	79
B. Composition and Geometric Perturbations.....	80
APPENDIX D .....	83
I. ERRORS ENCOUNTERED .....	83
II. REPEATED NUCLIDE TEST SET .....	84
A. Input File Rep01 .....	84
B. Input File Rep02 .....	84

C. Input File Rep03 .....	85
D. Input File Rep04 .....	85
E. Input File Rep09 .....	86
<b>APPENDIX E .....</b>	<b>89</b>
I. NEW TEST SUITE PROBLEM INP10 .....	89
II. NEW TEST SUITE PROBLEM INP11 .....	90
III. NEW TEST SUITE PROBLEM INP18 .....	92

## LIST OF FIGURES

Fig. 1. Godiva–Density Perturbation. Plotted results were calculated by MCNP4C.....	32
Fig. 2. Godiva–Composition Perturbation. Plotted results were calculated by MCNP4C. ....	34
Fig. 3. Test Problem INP18– $k_{\text{eff}}$ Estimate. Plotted results were calculated by MCNP4C. ....	35
Fig. 4. Test Problem INP02–Neutron Absorption Rate Estimate. Plotted results were calculated by MCNP4C. ....	36
Fig. 5. Test Problem INP04–Photon Collision Rate Estimate. Plotted results were calculated by MCNP4C. ....	38
Fig. 6. Test Problem INP10–Photon Collision Rate Estimate. Plotted results were calculated by MCNP4C. ....	40



## LIST OF TABLES

TABLE I:	Godiva Density Perturbation — $k_{\text{eff}}$ Estimate.....	32
TABLE II:	Godiva Composition Perturbation — $k_{\text{eff}}$ Estimate .....	33
TABLE III:	Test Problem INP18 — $k_{\text{eff}}$ Estimate .....	34
TABLE IV:	Test Problem INP02 — Neutron Absorption Rate Estimate .....	36
TABLE V:	Test Problem INP04 — Photon Collision Rate Estimate.....	37
TABLE VI:	Lithium Bin Uncorrected Perturbations.....	38
TABLE VII:	Test Problem INP10 — Photon Collision Rate Estimate.....	39



**VERIFICATION OF THE MCNP™ PERTURBATION CORRECTION  
FEATURE FOR CROSS-SECTION DEPENDENT TALLIES**

by

**A. K. Hess, J. S. Hendricks, G. W. McKinney, and L. L. Carter**

**ABSTRACT**

The Monte Carlo N-Particle Transport Code MCNP version 4B perturbation capability has been extended to cross-section dependent tallies and to the track-length estimate of  $k_{\text{eff}}$  in criticality problems. We present the complete theory of the MCNP perturbation capability including the correction to MCNP4B which enables cross-section dependent perturbation tallies. We also present the MCNP interface as an upgrade to the MCNP4B manual. Finally, we present test results demonstrating the validity of the perturbation capability in MCNP, particularly cross-section dependent problems.

## I. INTRODUCTION

The latest release of the Monte Carlo N-Particle Transport code (MCNP4B)<sup>1</sup> included a new perturbation feature not found in previous versions. This feature allows users, in a single run, to calculate the effects of perturbations to material composition or density. However, this useful capability was not valid in perturbed regions where the tally was dependent upon the material cross section since the differential operator technique was implemented.<sup>2</sup> Therefore, some tallies (such as reaction rate estimators, and track-length estimates for  $k_{\text{eff}}$ ) could not always be used with the perturbation feature and obtain accurate results.

The differential operator technique as developed by Gregg McKinney, was used to calculate the effect of perturbations on a tally.<sup>2</sup> This method was used since it allows the calculation of perturbations even if the standard deviation of the unperturbed tally is greater than the calculated perturbation. The differential operator technique was implemented using a second-order Taylor series expansion.

A derivation of the first- and second-order corrected perturbations was reported by Densmore, McKinney, and Hendricks.<sup>3</sup> This derivation allowed the user to determine a correction term which was to be added to the perturbation calculated by MCNP4B. The correction term accounts for the tally response estimator's dependence upon the perturbed cross-section data.<sup>3</sup> The correction term calculation has now been included as a capability of the perturbation feature for release in MCNP version 4C. This version no longer requires the tedious correction term calculation be performed by the user.

This report will detail the derivation of the corrected differential operator for the first two Taylor series coefficients. The theory is presented as a background for the verification work. Although it is documented in Refs. 2-5, this paper is the first documentation of the complete theory as used in MCNP that can be referenced. Following the theory section is a discussion of the PERT and FM cards. These cards are the user interface to the perturbation and correction capabilities. Finally, a discussion is presented about the testing and verification of the perturbation capability, emphasizing the new correction term capability. Appendix A includes input test files which were used for verification of the new capability. Appendix B contains the test files created by Densmore in Ref. 3 and used in this study for verification of the cross-section dependent tally capability. Appendix C includes example perturbation problems. Appendix D details the perturbation feature errors which were identified in version 4B of MCNP while testing the new version

4C. Appendix E contains the updated MCNP installation test suite problems which reflect the changes made to the perturbation capabilities.

## II. THEORY

This section details the derivation of the differential operator with the perturbation correction for cross-section dependent tallies for the  $n^{\text{th}}$  order Taylor series coefficient. It relies heavily upon the derivations given in LA-13098,<sup>2</sup> LA-13374,<sup>3</sup> X-6:GWM-94-124,<sup>4</sup> and XCI:JSH-98-99 (U) -rev. 1.<sup>5</sup>

### A. Derivation of the Operator

In the differential operator approach, a change in the Monte Carlo response  $c$ , due to changes in a related data set (represented by the parameter  $v$ ), is given by a Taylor series expansion

$$\Delta c = \frac{dc}{dv} \cdot \Delta v + \frac{1}{2!} \cdot \frac{d^2c}{dv^2} \cdot \Delta v^2 + \dots + \frac{1}{n!} \cdot \frac{d^n c}{dv^n} \cdot \Delta v^n + \dots ,$$

where the  $n^{\text{th}}$  order coefficient is

$$u_n = \frac{1}{n!} \cdot \frac{d^n c}{dv^n} . \quad (1)$$

For the data set

$$x_b(h) = K_b(h) \cdot e^v; \quad b \in B, h \in H , \quad (2)$$

$K_b(h)$  is some constant,  $B$  represents a set of macroscopic cross sections, and  $H$  represents a set of energies or an energy interval. By differentiating the data set, it is easily found that

$$\frac{d}{dv} x_b(h) = K_b(h) \cdot e^v = x_b(h) . \quad (3)$$

Using the chain rule and Eq. (2) and (3), Eq. (1) for  $u_n$  can be written as

$$\begin{aligned}
u_n &= \frac{1}{n!} \sum_{b \in B} \sum_{h \in H} \left( \frac{\partial^n c}{\partial x_b^n(h)} \right) \frac{\partial^n}{\partial v^n} x_b^n(h) \\
&= \frac{1}{n!} \sum_{b \in B} \sum_{h \in H} x_b^n(h) \left( \frac{\partial^n c}{\partial x_b^n(h)} \right). \tag{4}
\end{aligned}$$

For a track-based response estimator

$$c = \sum_i t_j q_j, \tag{5}$$

where  $t_j$  is the response estimator and  $q_j$  is the probability of path segment  $j$  (path segment  $j$  is comprised of segment  $j-1$  plus the current track). Substituting Eq. (5) into Eq. (4),  $u_n$  becomes

$$u_n = \frac{1}{n!} \sum_j \left[ \sum_{b \in B} \sum_{h \in H} x_b^n(h) \left( \frac{\partial^n}{\partial x_b^n(h)} (t_j q_j) \right) \right],$$

or

$$u_n = \frac{1}{n!} \sum_j \gamma_{nj} t_j q_j, \tag{6}$$

where

$$\gamma_{nj} \equiv \sum_{b \in B} \sum_{h \in H} x_b^n(h) \left( \frac{\partial^n}{\partial x_b^n(h)} (t_j q_j) \right) \left( \frac{1}{t_j q_j} \right). \tag{7}$$

When particle histories are sampled one track at a time, it is advantageous to have a perturbation operator that also operates on a track basis combined with an estimator that estimates for an entire particle history. In other words, Eq. (6) must be converted from a path segment estimator to a particle history estimator. To accomplish this, the variable  $\delta_{ij}$  is defined such that  $\delta_{ij} = 1$  if particle history  $i$  contains path segment  $j$  and zero otherwise. The probability of sampling particle history  $i$  from all particle histories containing path segment  $j$  is

$$\left( \frac{\delta_{ij} p_i}{q_j} \right) ,$$

where  $p_i$  is the probability of particle history  $i$ . One property of such a quantity is that

$$\sum_i \left( \frac{\delta_{ij} p_i}{q_j} \right) = 1 , \quad (8)$$

for all path segments. Multiplying Eq. (6) by Eq. (8) produces

$$\begin{aligned} u_n &= \frac{1}{n!} \sum_j \gamma_{nj} t_j q_j \cdot \sum_i \left( \frac{\delta_{ij} p_i}{q_j} \right) \\ &= \sum_i \left( \frac{1}{n!} \sum_j \delta_{ij} \gamma_{nj} t_j \right) p_i \\ &= \sum_i V_{ni} p_i , \end{aligned} \quad (9)$$

where  $V_{ni}$  is the  $n^{\text{th}}$  order coefficient estimator for history  $i$ , given by

$$V_{ni} \equiv \frac{1}{n!} \sum_{i'} \gamma_{nij'} t_{j'} . \quad (10)$$

Note the sum in Eq. (10) involves only those path segments  $j'$  in particle history  $i$ . The Monte Carlo expected value of  $u_n$  becomes

$$\begin{aligned} \langle u_n \rangle &= \frac{1}{N} \sum_i V_{ni} \\ &= \frac{1}{N n!} \sum_i \left( \sum_{j'} \gamma_{nij'} t_{j'} \right) , \end{aligned} \quad (11)$$

for a sample of  $N$  particle histories.

The probability of path segment  $j$  is the product of track probabilities

$$q_{j'} = \prod_{k=0}^m r_k , \quad (12)$$

where  $r_k$  is the probability of track  $k$  and segment  $j'$  contains  $m + 1$  tracks. If the  $k^{\text{th}}$  track starts with a neutron undergoing reaction type "a" at energy  $E'$  and is scattered from angle  $\theta'$  to angle  $\theta$ , and energy  $E$  continues for a length  $\lambda_k$  and collides, then

$$r_k = \left( \frac{x_a(E')}{x_T(E')} \right) P_a(E' \rightarrow E; \theta' \rightarrow \theta) dE d\theta (e^{-x_T(E)\lambda_k}) x_T(E) , \quad (13)$$

where  $x_a(E')$  is the macroscopic reaction cross section at energy  $E'$ ,  $x_T(E')$  is the total cross section at energy  $E'$ , and  $P_a(E' \rightarrow E; \theta' \rightarrow \theta) dE d\theta$  is the probability distribution function in phase space of the emerging neutron. If the track starts with a collision and ends in a boundary crossing

$$r_k = \left( \frac{x_a(E')}{x_T(E')} \right) P_a(E' \rightarrow E; \theta' \rightarrow \theta) dE d\theta (e^{-x_T(E)\lambda_k}) . \quad (14)$$

If the track starts with a boundary crossing and ends with a collision,

$$r_k = (e^{-x_T(E)\lambda_k}) x_T(E) .$$

And finally, if the track starts and ends with boundary crossings

$$r_k = e^{-x_T(E)\lambda_k} .$$

**1. First Order.** For a first-order perturbation, the differential operator becomes

$$\begin{aligned} \gamma_{1j'} &= \sum_{b \in B} \sum_{h \in H} x_b(h) \left( \frac{\partial}{\partial x_b(h)} (t_{j'} q_{j'}) \right) \left( \frac{1}{t_{j'} q_{j'}} \right) \\ &= \sum_{b \in B} \sum_{h \in H} \left( \frac{x_b(h) \partial q_{j'}}{q_{j'} \partial x_b(h)} + \frac{x_b(h) \partial t_{j'}}{t_{j'} \partial x_b(h)} \right) . \end{aligned} \quad (15)$$

Combining Eqs. (15) and (12) gives

$$\frac{1}{q_{j'} \partial x_b(h)} \frac{\partial q_{j'}}{\partial x_b(h)} = \sum_{k=0}^m \frac{1}{r_k \partial x_b(h)} \frac{\partial r_k}{\partial x_b(h)} , \quad (16)$$

then

$$\gamma_{1j'} = \sum_{k=0}^m \beta_{j'k} + R_{1j'} , \quad (17)$$

where

$$\beta_{j'k} \equiv \sum_{b \in B} \sum_{h \in H} \frac{x_b(h)}{r_k} \left( \frac{\partial r_k}{\partial x_b(h)} \right) , \quad (18)$$

and

$$R_{1j'} = \sum_{b \in B} \sum_{h \in H} \frac{x_b(h)}{t_{j'}} \left( \frac{\partial t_{j'}}{\partial x_b(h)} \right) . \quad (19)$$

Let  $r_k$  be divided into collision,  $C_k$ , and transport,  $Q_k$ , components where

$$C_k = \left( \frac{x_a(E')}{x_T(E')} \right) P_a(E' \rightarrow E; \theta' \rightarrow \theta) , \quad (20)$$

and

$$Q_k = e^{-x_T(E)\lambda_k} x_T(E) . \quad (21)$$

Then from Eq. (13),  $r_k = Q_k C_k$ , and

$$\frac{x_b(h) \partial r}{r_k \partial x} = \frac{x_b(h)}{Q_k C_k \partial x_b(h)} \frac{\partial}{\partial x_b(h)} [Q_k C_k] = \frac{x_b(h) \partial C_k}{C_k \partial x_b(h)} + \frac{x_b(h) \partial Q_k}{Q_k \partial x_b(h)} . \quad (22)$$

Whereas

$$\begin{aligned}
\frac{1}{C_k} \frac{\partial C_k}{\partial x_b(h)} &= \left( \frac{x_T(E')}{x_a(E')} \right) \frac{\partial}{\partial x_b(h)} \left[ \frac{x_a(E')}{x_T(E')} \right] \\
&= \left( \frac{x_T(E')}{x_a(E')} \right) \left( \frac{1}{x_T(E')} \delta_{hE} \delta_{ba} - \frac{x_a(E')}{x_T^2(E')} \delta_{hE'} \right) \\
&= \frac{\delta_{hE} \delta_{ba}}{x_b(E')} - \frac{\delta_{hE'}}{x_T(E')} ,
\end{aligned} \tag{23}$$

and

$$\begin{aligned}
\frac{\partial Q_k}{\partial x_b(h)} &= e^{-x_T(E)\lambda_k} (1 - x_T(E)\lambda_k) \delta_{hE} \\
&= e^{-x_T(E)\lambda_k} x_T(E) \left( \frac{1}{x_T(E)} - \lambda_k \right) \delta_{hE} .
\end{aligned} \tag{24}$$

Thus, by substitution of Eq. (21)

$$\frac{1}{Q_k} \frac{\partial Q_k}{\partial x_b(h)} = \left( \frac{1}{x_T(E)} - \lambda_k \right) \delta_{hE} . \tag{25}$$

Then combining Eqs. (18), (22), (23), and (25) gives

$$\beta_{j'k} = \sum_{b \in B} \sum_{h \in H} \left( \delta_{hE} \delta_{ba} - \frac{\delta_{hE} x_b(E')}{x_T(E')} - \delta_{hE} x_b(E) \lambda_k + \frac{\delta_{hE} x_b(E)}{x_T(E)} \right) , \tag{26}$$

for a track segment  $k$  that starts with a particle undergoing reaction type "a" at energy  $E'$  and is scattered to energy  $E$  and collides after a distance  $\lambda_k$ . Note that  $\delta_{hE}$  and  $\delta_{ba}$  are unity if  $h = E$  and  $b = a$ ; otherwise, they vanish. For other types of tracks (for which the various expressions for  $r_k$  were given in the previous section), i.e., collision to boundary, boundary to collision, and boundary to boundary, derivatives of  $r_k$  can be taken leading to one or more of these four terms for  $\beta_{j'k}$ .

The second term of  $\gamma_{1j'}$  in Eq. (17) is Eq. (19) which is

$$R_{1j'} = \sum_{b \in B} \sum_{h \in H} \frac{x_b(h)}{t_{j'}} \left( \frac{\partial t_{j'}}{\partial x_b(h)} \right) ,$$

where the tally response is a linear function of some combination of reaction cross sections, or

$$t_{j'} = \lambda_k \sum_{c \in C} x_c(E) , \quad (27)$$

where  $c$  is an element of the tally cross sections,  $c \in C$ , and may be an element of the perturbed cross sections,  $c \in B$ . Then substituting Eq. (27) into Eq. (19) gives

$$R_{1j'} = \sum_{b \in B} \sum_{h \in H} \frac{x_b(h)}{\lambda_k \sum_{c \in C} x_c(h)} \left( \frac{\partial}{\partial x_b(h)} \left[ \lambda_k \sum_{c \in C} x_c(h) \right] \right) ;$$

then, by performing the derivative and simplifying one finds

$$R_{1j'} = \frac{\sum_{c \in B} \sum_{E \in H} x_c(E)}{\sum_{c \in C} x_c(E)} . \quad (28)$$

The fraction of the reaction rate tally involved in the perturbation is  $R_{1j'}$ . If none of the nuclides participating in the tally is involved in the perturbation, then  $R_{1j'} = 0$ , which is always the case for F1, F2, and F4 tallies without FM cards. F1 tallies have  $R_{1j'} = 0$  since these are tallies of the current integrated over a surface and are independent of material cross sections. The same is true for F2 tallies since they tally the flux averaged over a surface. F4 tallies without an FM card also use  $R_{1j'} = 0$  since they tally the flux averaged over a cell, again a material independent value.

For F4 tallies with an FM card, if the FM card's multiplicative constant is positive (no flag to multiply by atom density), it is assumed that the FM tally cross sections are unaffected by the perturbation and  $R_{1j'} = 0$ . For KCODE  $k_{\text{eff}}$  track-length estimates, F6 and F7 heating tallies,

and F4 tallies with FM cards with negative multipliers (multiply by atom density to get macroscopic cross sections), if the tally cross section is affected by the perturbation, then  $R_{1j'} > 0$ . For  $k_{\text{eff}}$  and F6 and F7 tallies in perturbed cells where all nuclides are perturbed, generally  $R_{1j'} = 1$ .

Finally, the expected value of the first-order coefficient is

$$\langle u_1 \rangle = \frac{1}{N} \sum_i \left[ \sum_{j'} \left( \sum_{k=0}^m \beta_{j'k} + R_{1j'} \right) t_{j'} \right] .$$

**2. Second Order.** For a second-order perturbation, the differential operator becomes

$$\begin{aligned} \gamma_{2j'} &= \sum_{b \in B} \sum_{h \in H} \frac{x_b^2(h)}{t_{j'} q_{j'}} \left( \frac{\partial^2}{\partial x_b^2(h)} (t_{j'} q_{j'}) \right) \\ &= \sum_{b \in B} \sum_{h \in H} \frac{x_b^2(h)}{t_{j'} q_{j'}} \left( t_{j'} \frac{\partial^2 q_{j'}}{\partial x_b^2(h)} + 2 \frac{\partial q_{j'}}{\partial x_b(h)} \frac{\partial t_{j'}}{\partial x_b(h)} + q_{j'} \frac{\partial^2 t_{j'}}{\partial x_b^2(h)} \right) . \end{aligned} \quad (29)$$

Since  $t_{j'}$  is a linear function of  $x_b(h)$ , then the last term of Eq. (29) is

$$\frac{\partial^2 t_{j'}}{\partial x_b^2(h)} = 0 ,$$

The middle term of Eq. (29) is (from Eq. (16), (18), and (19))

$$\begin{aligned}
& \sum_{b \in B} \sum_{h \in H} \frac{2x_b^2(h) \partial q_{j'}}{t_{j'} q_{j'}} \frac{\partial t_{j'}}{\partial x_b(h)} \\
&= 2 \sum_{b \in B} \sum_{h \in H} \left( \sum_{k=0}^m \frac{x_b(h) \partial r_k}{r_k \partial x_b(h)} \right) \left( \frac{x_b(h) \partial t_{j'}}{t_{j'} \partial x_b(h)} \right) \\
&= 2R_{1j'} \sum_{k=0}^m \beta_{j'k} \\
&= \left( \sum_{k=0}^m \beta_{j'k} + R_{1j'} \right)^2 - \left( \sum_{k=0}^m \beta_{j'k} \right)^2 - R_{1j'}^2 .
\end{aligned} \tag{30}$$

This form is useful later and comes from  $2AB = (A+B)^2 - A^2 - B^2$ .

The first term of Eq. (29) is (utilizing Eq. (16))

$$\begin{aligned}
\frac{x_b^2(h) \partial^2 q_{j'}}{q_{j'} \partial x_b^2(h)} &= \frac{x_b^2(h)}{q_{j'}} \frac{\partial}{\partial x_b(h)} \left( q_{j'} \sum_{k=0}^m \frac{1}{r_k} \frac{\partial r_k}{\partial x_b(h)} \right) \\
&= \left( \sum_{k=0}^m \frac{x_b(h) \partial r_k}{r_k \partial x_b(h)} \right)^2 + x_b^2(h) \sum_{k=0}^m \frac{\partial}{\partial x_b(h)} \left( \frac{1}{r_k} \frac{\partial r_k}{\partial x_b(h)} \right) \\
&= \left( \sum_{k=0}^m \frac{x_b(h) \partial r_k}{r_k \partial x_b(h)} \right)^2 - \sum_{k=0}^m \left( \frac{x_b(h) \partial r_k}{r_k \partial x_b(h)} \right)^2 + \sum_{k=0}^m \frac{x_b^2(h) \partial^2 r_k}{r_k \partial x_b^2(h)} \\
&= \left( \sum_{k=0}^m \beta_{j'k} \right)^2 + \sum_{k=0}^m (\alpha_{j'k} - \beta_{j'k}^2) .
\end{aligned} \tag{31}$$

where the  $\alpha_{j'k}$  term is

$$\alpha_{j'k} = \sum_{b \in B} \sum_{h \in H} \frac{x_b^2(h) \partial^2 r_k}{r_k \partial x_b^2(h)} . \tag{32}$$

Substituting Eqs. (30) and (31) into Eq. (29) gives

$$\gamma_{2j'} = \sum_{k=0}^m (\alpha_{j'k} - \beta_{j'k}^2) - R_{1j'}^2 + \left( \sum_{k=0}^m \beta_{j'k} + R_{1j'} \right)^2. \quad (33)$$

The only additional work for calculating the 2<sup>nd</sup> order coefficient is evaluating  $\alpha_{j'k}$ . To solve for  $\alpha_{j'k}$ , let  $r_k = Q_k C_k$  as in Eqs. (13), (20), and (21). Then:

$$\begin{aligned} \frac{1}{r} \frac{\partial^2 r_k}{\partial x_b^2(h)} &= \frac{1}{Q_k C_k} \frac{\partial^2}{\partial x_b^2(h)} [Q_k C_k] = \frac{1}{Q_k C_k} \frac{\partial}{\partial x_b(h)} \left[ Q_k \frac{\partial C_k}{\partial x_b(h)} + C_k \frac{\partial Q_k}{\partial x_b(h)} \right] \\ &= \frac{1}{C_k} \frac{\partial^2 C_k}{\partial x_b^2(h)} + \frac{1}{Q_k} \frac{\partial^2 Q_k}{\partial x_b^2(h)} + \frac{2}{Q_k C_k} \left( \frac{\partial Q_k}{\partial x_b(h)} \right) \left( \frac{\partial C_k}{\partial x_b(h)} \right). \end{aligned} \quad (34)$$

To evaluate the 1<sup>st</sup> term of Eq. (34), take the derivative of  $\frac{x_a(E')}{x_T(E')}$  using Eq. (23)

$$\begin{aligned} \frac{\partial^2}{\partial x_b^2(h)} \left[ \frac{x_a(E')}{x_T(E')} \right] &= \frac{\partial}{\partial x_b(h)} \left[ \frac{1}{x_T(E')} \delta_{hE'} \delta_{ba} - \frac{x_a(E')}{x_T^2(E')} \delta_{hE'} \right] \\ &= - \left( \frac{1}{x_T(E')} \right)^2 \delta_{hE'} \delta_{ba} - \frac{1}{x_T^2(E')} \delta_{hE'} \delta_{ba} + 2 \left( \frac{x_a(E')}{x_T^2(E')} \right) \delta_{hE'} \\ &= \frac{x_a(E')}{x_T(E')} \left\{ \frac{(-2)(\delta_{hE'} \delta_{ba})}{x_a(E') x_T(E')} + \frac{2 \delta_{hE'}}{x_T^2(E')} \right\}. \end{aligned} \quad (35)$$

From Eq. (35) and the definition of  $C_k$  in Eq. (20), the 1<sup>st</sup> term becomes

$$\frac{1}{C_k} \frac{\partial^2 C_k}{\partial x_b^2(h)} = \frac{(-2)(\delta_{hE'} \delta_{ba})}{x_b(E') x_T(E')} + \frac{2 \delta_{hE'}}{x_T^2(E')}. \quad (36)$$

To evaluate the 2<sup>nd</sup> term of Eq. (34), take the derivative of Eq. (24)

$$\begin{aligned}
\frac{1}{Q_k} \frac{\partial^2 Q_k}{\partial x_b^2(h)} &= \frac{1}{Q_k} \frac{\partial}{\partial x_b(h)} \left[ e^{-x_T(E)\lambda_k} x_T(E) \left( \frac{1}{x_T(E)} - \lambda_k \right) \delta_{hE} \right] \\
&= \frac{e^{-x_T(E)\lambda_k}}{Q_k} \left\{ -\lambda_k (1 - x_T(E)\lambda_k) - \lambda_k \right\} \delta_{hE} \\
&= \left( \frac{-2\lambda_k}{x_T(E)} + \lambda_k^2 \right) \delta_{hE} \\
&= \frac{-2\lambda_k \delta_{hE}}{x_T(E)} + \lambda_k^2 \delta_{hE}
\end{aligned} \tag{37}$$

The 3<sup>rd</sup> term of Eq. (34) is simply two times the product of Eqs. (23) and (25)

$$\frac{2}{Q_k C_k} \left( \frac{\partial Q_k}{\partial x_b(h)} \right) \left( \frac{\partial C_k}{\partial x_b(h)} \right) = 2 \left( \frac{\delta_{hE'} \delta_{ba}}{x_b(E')} - \frac{\delta_{hE'}}{x_T(E')} \right) \left( \frac{\delta_{hE}}{x_T(E)} - \lambda_k \delta_{hE} \right) \tag{38}$$

Substituting Eqs. (36), (37), and (38) in to Eq. (34), then Eq. (32) becomes

$$\begin{aligned}
\alpha_{j'k} &= \sum_{b \in B} \sum_{h \in H} \left( \frac{2\delta_{hE'} x_b^2(E')}{x_T^2(E')} - \frac{2\delta_{hE'} \delta_{ba} x_b(E')}{x_T(E')} + \delta_{hE} x_b^2(E) \lambda_k^2 + \frac{2\delta_{hE} x_b^2(E) \lambda_k}{x_T(E)} \right. \\
&\quad \left. + 2 \left( \delta_{hE'} \delta_{ba} - \frac{x_b(E') \delta_{hE'}}{x_T(E')} \right) \left( \frac{x_b(E) \delta_{hE}}{x_T(E)} - \lambda_k \delta_{hE} x_b(E) \right) \right) \tag{39}
\end{aligned}$$

The expected value of the second-order coefficient is

$$\langle u_2 \rangle = \frac{1}{2N} \sum_i \left[ \sum_{j'} \left( \sum_{k=0}^m (\alpha_{j'k} - \beta_{j'k}^2) - R_{1j'}^2 + \left( \sum_{k=0}^m \beta_{j'k} + R_{1j'} \right)^2 \right) t_{j'} \right] ,$$

where  $\beta_{j'k}$  and  $\alpha_{j'k}$  are given by one or more terms as described above for track  $k$  and  $R_{1j'}$  is again the fraction of the perturbation with nuclides participating in the tally.

## B. Implementation in MCNP

The total perturbation printed in the MCNP output file is

$$\langle \Delta c \rangle = \frac{1}{N} \sum_i \sum_{i'} \Delta c_{j'} .$$

For each history  $i$  and path  $j'$ ,

$$\Delta c_{j'} = \frac{dc_{j'}}{dv} \cdot \Delta v + \frac{1}{2} \cdot \frac{d^2 c_{j'}}{dv^2} \cdot \Delta v^2 .$$

Let the first-order perturbation with  $R_{1j'} = 0$  be

$$P_{1j'} = \sum_{j'} \left( \sum_{k=0}^m \beta_{j'k}^2 \right) t_{j'} ,$$

and let the second-order perturbation with  $R_{1j'} = 0$  be

$$P_{2j'} = \sum_{j'} \left( \sum_{k=0}^m \alpha_{j'k} - \beta_{j'k}^2 \right) t_{j'} .$$

Then the Taylor series expansion for  $R_{1j'} = 0$  is

$$\Delta c_{j'} = \left( P_{1j'} \Delta v + \frac{1}{2} (P_{2j'} + P_{1j'}^2) \Delta v^2 \right) t_{j'} .$$

If  $R_{1j'} \neq 0$  then

$$\begin{aligned} \Delta c_{j'} &= \left( (P_{1j'} + R_{1j'}) \Delta v + \frac{1}{2} (P_{2j'} - R_{1j'}^2 + (P_{1j'} + R_{1j'})^2) \Delta v^2 \right) t_{j'} \\ &= \left[ P_{1j'} \Delta v + \frac{1}{2} (P_{2j'} + P_{1j'}^2) \Delta v^2 + R_{1j'} \Delta v + P_{1j'} R_{1j'} \Delta v^2 \right] t_{j'} . \end{aligned}$$

That is, the  $R_{1j'} \neq 0$  case is just a correction to the  $R_{1j'} = 0$  case.

In MCNP,  $P_{1j'}$  and  $P_{2j'}$  are accumulated along every track length through a perturbed cell. All perturbed tallies are multiplied by

$$\left( P_{1j'} \Delta v + \frac{1}{2} (P_{2j'} + P_{1j'}^2) \Delta v^2 \right) ,$$

and then if  $R_{1j'} \neq 0$  the tally is further corrected by

$$R_{1j'} \Delta v + (P_{1j'} R_{1j'}) \Delta v^2 .$$

The fraction of the reaction rate tally involved in the perturbation is  $R_{1j'}$ .  $R_{1j'} = 0$  for F1, F2, F4 tallies without FM cards, and F4 tallies with FM cards with positive multiplicative constants. The new cross-section dependent tally term is automatically calculated in MCNP4C for F4 tallies using negative multiplicative constants on corresponding FM cards; it is also automatically calculated for F6, F7, and  $k_{\text{eff}}$  problems. This calculation was omitted in MCNP4B making perturbed tallies wrong when  $R_{1j'} > 0$ .

### III. USER INTERFACE

The input card used to utilize the perturbation feature is the PERT card. The following sections give a description of the parameters, abilities, limitations, and new additions to the PERT and FM interfaces. In the first few sections, we repeat much of what can be found in the MCNP4B users manual<sup>1</sup> and in LA-13098.<sup>2</sup>

#### A. PERT Card

The PERT card is the MCNP user interface to the perturbation feature. The following sections describe its general usage and the options available when using this card.

**1. General Description.** The PERT card allows perturbations in cell material density, composition or reaction cross-section data. The perturbation analysis uses the first and second-order differential operator technique described in Section II of this report. Using this technique, the perturbation estimates are made without actually changing the input material specifications.

Multiple perturbations can be applied in the same run, each specified by a separate PERT card. There is no limit to the number of perturbations which can be used. The entire tally output is repeated for each perturbation, giving the estimated differential change in the tally, or this change can be added to the unperturbed tally (see METHOD keyword below). The number of tallies and perturbations should be kept to a minimum due to increased running time and output associated with the perturbation feature. A track-length estimate of perturbations to  $k_{\text{eff}}$  is automatically estimated and printed for KCODE problems. The CELL keyword that identifies one or more perturbed problem cells is required. Also, either the MAT or RHO keyword must be specified.

Form: **PERTn:pl** keyword=parameter(s) keyword=parameter(s) ...

n = Unique, arbitrary perturbation number.  
pl = N or P or N,P. Not available for electrons.  
keyword = See the following section.

**2. PERT Card Keywords.** Six keywords are available for the PERT card. The CELL keyword and either the MAT or RHO keywords are required. The keywords are described as follows:

**CELL** - The one or more entries following this keyword indicate which cells are perturbed. At least one entry is required, and there is no limit to the number of entries. A comma or space delimiter is required between entries:

CELL=1,2,3,4

CELL=1 10i 12

**MAT** - The entry following this keyword specifies the perturbation material number, which must have a corresponding M card. Composition changes can only be made through the use of the MAT keyword. If the RHO keyword is omitted, the MAT keyword is required. Note in Section III.D that certain composition changes are prohibited.

**RHO** - Specifies the perturbed density of the cell(s) listed after the CELL key-

word. A positive entry indicates units of atoms/barn-cm and a negative entry grams/cm<sup>3</sup>. If the MAT keyword is omitted, the RHO keyword is required.

**METHOD** - This keyword specifies the number of terms to include in the perturbation estimate:

- 1 - include first and second order (default)
- 2 - include only first order
- 3 - include only second order

A positive entry produces perturbation tallies which give the estimated *differential* change in the unperturbed tally (default). A negative entry generates perturbation tallies such that this change is *added* to the unperturbed tally. The ability to produce first- and second-order terms separately enables the user to determine the significance of including the second-order estimator for subsequent runs. If the second-order results are a significant fraction (20%) of the total perturbation, then higher order terms are necessary to predict accurately the change in the unperturbed tally. In such cases, the magnitude of the perturbation should be reduced to satisfy this condition. Typically, this technique is accurate to within a few percent for up to 30% changes in the unperturbed tally.

**ERG** - The two entries following this keyword specify an energy range in which the perturbation is applied. The default range includes all energies. The ERG keyword is usually used with the RXN keyword to perturb a specific cross section over a particular energy range.

**RXN** - Entries following this keyword must be ENDF/B reaction types that identify one or more cross sections to perturb. The RXN keyword allows the user to perturb a single reaction cross section of a single nuclide in a material, all reaction types of a single nuclide, a single reaction for all nuclides in a material, and a set of cross sections for all nuclides in a material. The default reaction is the total cross section (RXN=1 for neutrons and multigroup, RXN=-5 for photons.) A list of

available reaction types is given in Appendix G of Ref. 1. Some non-standard special reaction numbers (see Section III.B.2) may also be used. Those which cannot be used include -4, -5, -7, and -8 for neutrons; -6 for photons; and -3, -4, -6, and -7 for multigroup problems.

## B. FM Card

The FM card is the MCNP user interface called the tally multiplier. It allows the user to create bins of tally responses to multiplicative and/or additive functions. The following sections describe the normal usage of the card and available reactions.

**1. Description of the FM Card.** The FM card is used to calculate a quantity of the form

$$C \int \varphi(E) R_m(E) dE ,$$

where  $\varphi(E)$  is the energy-dependent fluence (particles / cm<sup>2</sup>) and  $R(E)$  is an operator of additive and/or multiplicative response functions from the MCNP cross-section libraries or specially designated quantities. Note that some MCNP cross-section library reaction numbers are different from ENDF/B reaction numbers. See Section III.B.2.

Form: FMn (bin set 1) (bin set 2) ... T

n = tally number  
 (bin set i) = ((multiplier set 1) (multiplier set 2) ... (attenuator set))

T = absent for no total over bins  
 = present for total over all bins

attenuator set = C -1 m<sub>1</sub> px<sub>1</sub> m<sub>2</sub> px<sub>2</sub> ...

multiplier set i = C m (reaction list 1) (reaction list 2) ...

special multiplier set i = C -k

C = multiplicative constant  
 -1 = flag indicating attenuator rather than multiplier set

m	= material number identified on Mm card
px	= density times thickness of attenuating material; atom density if positive, mass density if negative
k	= special multiplier option:
(reaction list i)=	sums and products of ENDF or special reaction numbers

The constant C may be any arbitrary scalar quantity that can be used for normalization. It also may be flagged negative (as is usually the case) to use macroscopic cross sections which may be dependent upon perturbed cross sections. The material number m must appear on an Mm card, but need not be used in a geometrical cell of the problem. A reaction list consists of one or more reaction numbers delimited by spaces and/or colons. A space between reaction numbers means multiply the reactions. A colon means add the reactions. The hierarchy of operation is to multiply first and then add. One bin is created for each reaction list. Thus, if  $R_1$ ,  $R_2$ , and  $R_3$  are three reaction numbers, the form  $R_1 R_2 : R_3$  represents one reaction list (one bin) calling for reaction  $R_3$  added to the product of reactions  $R_1$  and  $R_2$ . No parentheses are allowed within the reaction list if a single bin is desired. The product of  $R_1$  with the sum of  $R_2$  and  $R_3$  would be represented by the form  $R_1 R_2 : R_1 R_3$  rather than by the form  $R_1 ( R_2 : R_3 )$ . The latter form would produce two bins with quite a different meaning.

The reaction cross sections are microscopic (with units of barns) and not macroscopic. Thus, if the constant C is the atomic density (in atoms per barn-cm), the results will include the normalization "per cm<sup>3</sup>." More often, C is flagged negative to convert to macroscopic cross sections and properly calculate perturbation cross-section dependency. See Section III.C.

**2. Reaction Numbers.** The reaction list on the FM card allows the use of most of the approximately one hundred standard ENDF reaction numbers available. There are, in addition, some nonstandard special reaction numbers that can be used. These are listed as follows:

- Neutrons:- 1 total cross section without thermal
- 2 absorption cross section
- 3 elastic cross section without thermal
- 4 average heating number (MeV / collision)

-5 Gamma-ray production cross section (barns) \*

-6 total fission cross section

-7 fission  $\nu$  \*

-8 fission Q (MeV / fission) \*

Photons: -1 incoherent scattering cross section

-2 coherent scattering cross section

-3 photoelectric cross section

-4 pair production cross section

-5 total cross section

-6 photon heating number \*

Multigroup:-1 total cross section

-2 fission cross section

-3 nubar data \*

-4 fission chi data \*

-5 absorption cross section

-6 stopping powers

-7 momentum transfers

A summary list of commonly used ENDF reactions can be found in Appendix G of the MCNP manual.<sup>1</sup>

### C. Perturbation Correction Capability for Cross-Section Dependent Tallies

The FM card may make a tally linearly dependent upon a cross section. If that cross section is perturbed in the same cell, then the perturbed tally may be dependent on the perturbed cross section. The dependency results in an extra term,  $R_{1j'}$ , (see Sections II.A.1 and 2) in the perturbation coefficients of the tally.  $R_{1j'}$  was not calculated in MCNP4B, which limited the usefulness of the PERT card in that version. In MCNP4C,  $R_{1j'}$  is computed automatically for PERT problems using F6 and F7 heating tallies, for  $k_{\text{eff}}$  track-length estimators, and for F4 track-length tallies with FM cards using a negative multiplicative constant ( $C < 0$ ). If  $C > 0$  then the FM card cross sections are microscopic and unconditionally assumed independent of any cross-section perturbation. However, if  $C < 0$ , then the FM card cross section is multiplied by  $|C|\rho_a$ , where

\* This reaction type may not be used to specify a RXN reaction on the PERT card.

$\rho_a$  is the atom density. The FM card cross sections are now macroscopic,  $\Sigma = \rho_a \sigma$ , dependency upon perturbed cross sections is now assumed possible, and  $R_{1j'}$  is calculated.

#### D. Perturbation and Correction Cautions

Although it is always a high priority to minimize the limitations of any MCNP feature, the perturbation technique itself, in addition to the numerous other MCNP features, resulted in the following limitations:

1. A fatal error is generated if a PERT card attempts to unvoid a region. The simple solution is to include the material in the unperturbed problem and void the region of interest with the PERT card (see Appendix C Section I.A for more details).
2. A fatal error is generated if a PERT card attempts to alter a material composition in such a way as to introduce a new nuclide. The solution is to set up the unperturbed problem with a mixture of both materials and introduce PERT cards to remove each (see Appendix C Section I.B for more details).
3. The track-length estimate of  $k_{\text{eff}}$  in KCODE criticality calculations assumes the fundamental eigenvector (fission distribution) is unchanged in the perturbed configuration.
4. Use caution in selecting the multiplicative constant and reaction number on FM cards used with F4 tallies in perturbation problems. The track-length correction term ( $R_{1j'}$  in Section II.A.1) is made only if the multiplicative constant on the FM card is negative (also indicating macroscopic cross sections due to multiplication by the atom density of the cell). If the multiplicative constant on the FM card is positive, it is assumed that any FM card cross sections are independent of the perturbed cross sections. If there is a reaction (RXN) specified on the PERT card, the track-length correction term,  $R_{1j'}$ , is only set if the exact same reaction is specified on the FM card. Synonymous reaction numbers are not equivalent in this case. For example, an entry of RXN=2 on the PERT card of a neutron problem is not equivalent to the special elastic reaction -3 on the FM card even though they both denote the elastic scattering cross section (one should either use 2 and 2 or -3 and -3).

5. DXTRAN, point detector tallies, and pulse height tallies are not currently compatible with the PERT card.
6. While there is no limit to the number of perturbations, they should be kept to a minimum, as each perturbation can degrade performance by 10-20%.
7. A fatal error is generated if the RXN parameter is specified on a mixed particle PERT card (i.e., PERT:n,p). This is due to the different MT and FM reaction numbers between particle types and the requirement of having the exact same reaction numbers on the FM and PERT cards (see caution 4).

## IV. CAPABILITY VERIFICATION

Extending the perturbation capability to cases where perturbed tallies depend upon perturbed cross sections required additional MCNP testing. The following sections describe those features and parameters of the PERT card which were tested and any verification efforts required to ensure correctness of the capability.

### A. Validation of MT Versus FM Reaction Numbers

A set of test problems was generated to verify that perturbations using the same reaction gave the same results regardless of whether MT or FM reaction numbers were specified. For instance, the MT and FM reaction numbers for the photon total microscopic cross section are 501 and -5 respectively (see Ref. 1 Appendix G). Either of these two reaction numbers can be specified on the PERT card. By using RXN=501, the results should match those obtained by RXN=-5. Also, this test set verifies that the default (no RXN parameter used or left blank on the PERT card) yields the expected perturbation. As stated in Section III.A.2 under the RXN keyword explanation, the default reaction is the total cross section: RXN=1 for neutrons and multigroup, and RXN=-5 for photons.

The “mtfm##” test set was created to check all synonymous MT and FM reactions. The files of this test set can be found in Appendix A, Section II.A. These tests resulted in identical tallies (as expected) whether using the MT or FM reaction number for the RXN parameter. Several of the problems used for testing MT versus FM reaction numbers were KCODE problems. The effect of the perturbation on the estimated track-length  $k_{\text{eff}}$  was found to exactly match between perturbations using MT and equivalent FM reaction numbers.

A fatal error is generated if an invalid nonstandard special reaction number is used. These reactions should not be perturbed by the user; when they are, the following error message results: “fatal error. reaction # invalid in perturbation #.” As stated in Section III.A.2, the invalid reactions for the RXN keyword are: -4, -5, -7, and -8 for neutrons; -6 for photons; and -3, -4, -6, and -7 for multigroup problems.

During the testing of MCNP4C, some errors were identified in MCNP4B. These errors have been corrected in version 4C and are documented in Appendix D.

## B. Neutron and Photon Perturbation with Specified RXN

For the case of a mixed particle PERT card (i.e., PERT:n,p), no RXN specification on the PERT card is allowed. This is due to the different MT and FM reaction numbers between particles and the requirement of having identical reaction specifications on the PERT and FM cards. For instance, neutrons have a total cross-section MT number of 1, whereas for photons, the same specification number is 501. Therefore, a fatal error occurs when such a specification is encountered. The error reads: “fatal error. rxn option and n,p option incompatible, perturbation #”.

## C. Lists of RXN Numbers

The “lis##” set tested lists of numbers used for the RXN parameter. These lists are matched exactly as on the FM card. (Mismatching MT and FM reaction numbers will not accurately perform the perturbation or correction, e.g., for neutrons a -3 on the FM card will not work with a 2 for RXN on the PERT card even though they both denote the elastic cross section.) Comparisons were made between a type 4 tally with an FM card using the FM number and another type 4 tally with an FM card using the equivalent sum of reactions as listed in Appendix G of Ref. 1. For example, “lis01” contains the following tally, FM, and PERT cards.

```
f4:n 1
f14:n 1
fm4 -1 1 -6
fm14 -1 1 19:20:21:38
pert1:n cell=1 rho=0.047 method=-1 rxn=-6
pert2:n cell=1 rho=0.047 method=-1 rxn=19 20 21 38
```

If the reaction list ability on the RXN parameter is operating correctly, one would expect these tallies to give identical results. Such a problem also validates self-consistency since the total fission cross section consists of the sum of reactions 19, 20, 21, and 38. A photon problem was generated using this same principle of checking the RXN list option. Both input files did produce matching tallies and are shown in Appendix A Section II.B.

#### D. Nonsequentially Numbered Cells

By not using sequentially numbered cells, MCNP must create its own reference cell numbering. This test was used to check that the perturbation feature still perturbed the correct cell. First, an input file was created which contained illogically numbered cells. Then an identical file was generated except the cells and all references to those cells were renumbered sequentially. A pair of input files for tests on neutrons and photons are included in Appendix A, Section II.C. If the perturbation feature works correctly with the nonsequentially numbered cells, the output results from both files should match as was the case.

The following is a highlight of the cell, surface, tally, and perturbation definitions.

```
mis01:  1   1  0.0479813   -1
        15  1  0.0479813   1  -215 -216  217
        4   1  0.0479813  -23  (215: 216 : -217)
        37  0           23

        1   so   2
        215 cx   3
        16  px   5
        217 px  -4
        23  so   8

f4:n  1
f14:n 15
f24:n  4
fm4 -1 1 -6 -7
fm14 -1 1 -6 -7
```

```

fm24 -1 1 -6 -7
pert1:n cell=1 mat=2 method=1 rxn= -6
pert4:n cell=4 mat=2 method=-1 rxn= -6
mis01b: 1 1 0.0479813 -1
          2 1 0.0479813 -2 (3: 4 : -5)
          3 1 0.0479813 1 -3 -4 5
          4 0           2

          1 so 2
          2 so 8
          3 cx 3
          4 px 5
          5 px -4

f4:n 1
f14:n 3
f24:n 2
fm4 -1 1 -6 -7
fm14 -1 1 -6 -7
fm24 -1 1 -6 -7
pert1:n cell=1 mat=2 method=1 rxn= -6
pert4:n cell=2 mat=2 method=-1 rxn= -6

```

## E. Positive and Negative RHO Numbers

This set was used to be certain that both positive and negative values for the PERT card RHO parameter were correct. Recall that a positive RHO indicates the units of atoms/cm<sup>3</sup> whereas a negative one denotes g/cm<sup>3</sup>. The problem rho01 uses two PERT cards, one with a density change in atoms/cm<sup>3</sup> (and denoted positively on the RHO parameter), and the second with the corresponding material density in g/cm<sup>3</sup>. The two perturbations generated the expected results of agreeing tallies. The entire file can be found in Appendix A Section II.D. The following lines show the important definitions in the file rho01.

rho01: f4:n 1

```
fm4 -1 1 1
pert1:n cell=1 rho=-18.7399 method=-1 rxn=1
pert2:n cell=1 rho=0.0479813 method=-1 rxn=1
```

This problem utilized the KCODE card. Both perturbed estimates (positive and equivalent negative rho values) of the track-length  $k_{\text{eff}}$  gave identical answers.

#### F. Bogus RXN, CELL, MAT, and METHOD Numbers

The bogus set was created to test the response of MCNP4C to bad numbers for the various parameters. Since the results are expected to be incorrect, these tests were not compared to any previous or subsequent runs for correctness. Alternatively, it was important to know how the new version of MCNP would respond so that the user could know what to expect if an erroneous option specifier is used. The following sections detail the options tested and the results obtained. Each of the described input files is given in its entirety in Appendix A Section II.E.

**1. Neutron Problem with Photon Reaction on RXN Parameter.** For a neutron KCODE problem, the default neutron reaction was specified on the corresponding FM card; however, the default photon reaction number was given on the RXN parameter of the PERT card. MCNP4C generated perturbed tally output which matched the unperturbed tally response. In short, no perturbation was applied, and the only warning given during execution was that of reaction 501 not being present in the specified library. The following lines detail the important features of this input file.

```
bog01: f4:n 1
        fm4 -1 1 1
        pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=501
```

**2. Unknown Reaction on RXN Parameter.** This neutron problem used a completely imagined reaction of 952 for the RXN parameter. Results are as in the above problem, no perturbation is applied, and the run-time warning is given stating that reaction 952 is not present in the specified library. The following lines detail the important features of this input file.

```
bog02:          f4:n 1
                  fm4 -1 1 1
                  pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=952
```

**3. Use of Nonexisting Cell on CELL Parameter.** Recall from Section III.A.2 that this parameter is required. If a cell number for a nonexistent cell is used on this parameter, a fatal error results stating: “fatal error. pert cell entry # is not a valid cell” where # is the nonexistent cell number specified on the CELL parameter. The following lines detail the cell and perturbation cards which are specified in this input file.

```
bog03:          1 1 0.0479813 -1
                  2 0          1
                  pert2:n cell=3 rho=-18.74 mat=2 method=-1 rxn=1
```

**4. Use of Nonexisting Material on MAT Parameter.** If a material number for a nonexistent material is used with the MAT parameter on the PERT card, a fatal error results stating: “fatal error. material # invalid for perturbation n” where # is the nonexistent material number specified on the MAT parameter, and n is the perturbation number on which it resides. The following lines detail the material and perturbation cards which are specified in this input file.

```
bog04:          m1 92235.50c -94.73 92238.50c -5.27
                  m2 92235.50c -87   92238.50c -13
                  pert2:n cell=1 rho=-18.74 mat=4 method=-1 rxn=1
```

**5. Use of Invalid Number on METHOD Parameter.** Recall from Section III.A.2 that the values of  $\pm 1$ ,  $\pm 2$ , and  $\pm 3$  are the only valid numbers that can be used for the METHOD parameter. This problem used METHOD=5 and resulted in a fatal error which reads, “fatal error. illegal method value.” The following line shows the PERT card used for this input problem.

```
bog05:          pert2:n cell=1 rho=-18.74 mat=2 method=5 rxn=1
```

**6. Bogus Parameter Findings.** From the two files of Sections IV.F.1 and 2, it can be seen that MCNP4C will warn the user of an unknown reaction type but will continue to report a number (the unperturbed tally results) for the perturbed tally. The user should take caution in believing perturbed tally results if the run-time warning is given. When nonexistent cells or materials are used, or if an invalid method number is used, a fatal error will result.

These tests were based upon a KCODE problem. Those problems which did not yield a fatal error (and thus stop all further calculations) reported perturbed tallies and track-length  $k_{eff}$  estimates. As stated before, the tallies reported the unperturbed response. However, the track-length  $k_{eff}$  estimates for the perturbation were not identical to the unperturbed ones. The estimates were within their statistical uncertainty, though.

## G. Energy Ranges Via the ERG Parameter

In order to test the ERG parameter, it was first necessary to determine an energy range in which no reaction change is expected. For this, the (n,2n) and (n,3n) reactions in material 92235.50c were used. They each have a threshold energy, (n,2n) at approximately 5.2 MeV and (n,3n) at approximately 11 MeV. Perturbing a tally on the sum of these two reactions should exhibit no difference from the unperturbed tally on just the (n,2n) reaction if the perturbation is below 11 MeV. Likewise, the sum of several reactions including the (n,2n) and (n,3n) reactions should show no change if perturbed below 5.2 MeV. In tests "erg01" and "erg02", one perturbation with the reaction(s) in question is compared to another perturbation without the reaction(s). The full input files are shown in Appendix A, Section II.F, but highlights of the source, tally, FM, and perturbation definitions are shown here. The perturbed tally results match exactly for a given problem.

```
erg01: sdef erg=d1 pos=0 0 0
       si1 L7
       sp1 1
       nonu
       f4:n 1
       fm4 -1 1 16:17
       f14:n 1
       fm14 -1 1 16
       pert1:n cell=1 rho=0.04 method=1 rxn=16 17 erg=5.5,9
       pert2:n cell=1 rho=0.04 method=1 rxn=16    erg=5.5,9
```

```
erg02: sdef erg=d1 pos=0 0 0
       si1 L5
```

```

sp1 1
nonu
f4:n 1
fm4 -1 1 -6:-3:16:17
f14:n 1
fm14 -1 1 -6:-3
pert1:n cell=1 rho=0.04 method=-1 rxn=-6 -3 16 17 erg=5.5,9
pert2:n cell=1 rho=0.04 method=-1 rxn=-6 -3          erg=5.5,9

```

In erg03, a KCODE problem was used to determine if the ERG option still perturbed the tally when the neutrons were allowed to range the energy spectrum. The two tallies, f4 and f14, do not match because some of the neutrons fall in the range of the (n,3n) reaction (above 11.5 MeV). However, the perturbed tallies and the effect of the perturbations on the track-length estimates did match, exactly. This match is expected because in the range of the 5.5 to 9 MeV there is no (n,3n) reaction to perturb.

```

erg03:  kcode 1000 1.0 10 40
        ksrc 0 0 0
        f4:n 1
        fm4 -1 1 16:17
        f14:n 1
        fm14 -1 1 16
        pert1:n cell=1 rho=0.04 method=1 rxn=16 17 erg=5.5,9
        pert2:n cell=1 rho=0.04 method=1 rxn=16    erg=5.5,9

```

## H. Effect on Other Tally Types

With a change in the perturbation calculations within MCNP4C, some simple tests were done to be certain that no undesirable effects occur when these changes are used in conjunction with other tally types. For tally types 1, 2, and 4 with no FM card, the results should track those from MCNP version 4B. This was found to be the case when MCNP4C was run on the version 4B test suite. No unexpected differences were found in the mctal or output files which confirms that the other tally types are not affected by the changes in the new version.

More definitive tests were performed on type 6 and 7 tallies since the new perturbation correction term applies. First, a problem was set up using only a type 6 or 7 tally ("tal6#" or "tal7#"). Then the problem was copied, and the 6 or 7 tally was substituted by an equivalent type 4 tally and FM card ("tal6#b" or "tal7#b"). Also, a very small density perturbation was added to perturb from a density slightly different from the tally 6 (or 7) run to the same density as the tally 6 (or 7) run. Both problems were then run to convergence to ensure that the perturbation correction is applied to the f6 (or f7) tally automatically. It was found that the perturbation correction is applied, and the perturbed result of "tal##b" does converge to the unperturbed result in "tal##". The KCODE problems (tal61, tal62, and tal71) were also found to yield estimates for track-length  $k_{eff}$  which converged to the expected results of the paired file.

Test files were generated for neutron, photon, neutron & photon, and multigroup type 6 tally tests. For a type 7 tally, only a neutron problem was generated because the type 7 tally is only valid for neutrons. All of these type 6, type 7, and equivalent perturbed f4 tally problems are included in Appendix A Section II.G. The important features of one pair of test files are shown below.

tal61: 1 1 0.0479813 -1  
2 0 1

kcode 1000 1.0 10 300  
ksrc 0 0 0  
f6:n 1

tal61b: 1 1 0.0485 -1  
2 0 1

kcode 1000 1.0 10 800  
ksrc 0 0 0  
f4:n 1  
fm4 -1 1 -1 -4  
pert1:n cell=1 rho=0.0479813 method=-1 rxn=-1

## V. FURTHER CROSS-SECTION-DEPENDENT TALLY VERIFICATION TESTS

The theory for cross-section-dependent tallies was originally presented in Ref. 3. By the use of six test problems, that study verified the method of correcting perturbed tallies for cross-section changes made by perturbations. These problems were used to compare actual MCNP results for an unperturbed problem to the results from a perturbed problem with the method applied. In this section, these test problems are run using MCNP4C with the correction applied via a negative multiplicative constant on the FM card. These results are then compared to those obtained earlier in Ref. 3. All reported errors in this section are given as standard deviations as was done in Ref. 3. The reported actual results were calculated by MCNP4C, but all match (within statistics) the actual results obtained by Densmore et al.

Each example contains five files, one containing four perturbations (approximately a 5%, 10%, 20%, and 30% change in the unperturbed tally). The other four files calculate the “actual” results which are found by establishing a problem that uses one perturbation’s characteristics for the problem. All files for each example of this test set can be found in Appendix B.

### A. Godiva–Density Perturbation

The KCODE problem “godiva1” perturbs the density of the Godiva critical assembly, an unreflected sphere of highly enriched uranium. The density was increased from  $18.74 \text{ g/cm}^3$  to  $26 \text{ g/cm}^3$ , and a track-length estimate of  $k_{\text{eff}}$  was calculated by the use of an F4 tally with an appropriate tally multiplier card. The unperturbed value for  $k_{\text{eff}}$  was  $0.998063 \pm 0.000798$ . Table I gives the predicted and actual results from MCNP4C for this problem and the predicted results from Ref. 3. The MCNP4C results are also graphed in Fig. 1.

As can be seen in Table I, the predicted values match the actual values, within statistics, up to about 5%. After this point the second-order perturbation underestimates  $k_{\text{eff}}$ . This bias is due to the inability of the differential operator, as implemented in MCNP, to calculate perturbed eigenfunctions. Essentially, the calculation of the perturbed eigenvalue is based on the eigenfunction at  $18.74 \text{ g/cm}^3$ .

Table I also provides an easy comparison between results obtained by MCNP4C and those found by calculating the perturbation cross-section dependency by the method described in Ref. 3. With much less user effort, the corrected tallies were found to match (within statistics) those which were calculated by Densmore et al.

TABLE I: Godiva Density Perturbation —  $k_{\text{eff}}$  Estimate

Density ( $\text{g}/\text{cm}^3$ )	MCNP4C Percent Change (Predicted)	MCNP4C Standard Deviation	Ref.3 Percent Change (Predicted)	Ref. 3 Standard Deviation	Percent Change (Actual)	Standard Deviation (Actual)
20	5.282	0.015	5.283	0.016	5.499	0.116
21	9.302	0.028	9.304	0.088	9.467	0.111
23.5	18.683	0.063	18.696	0.059	19.389	0.117
26	27.110	0.103	27.142	0.093	28.256	0.122

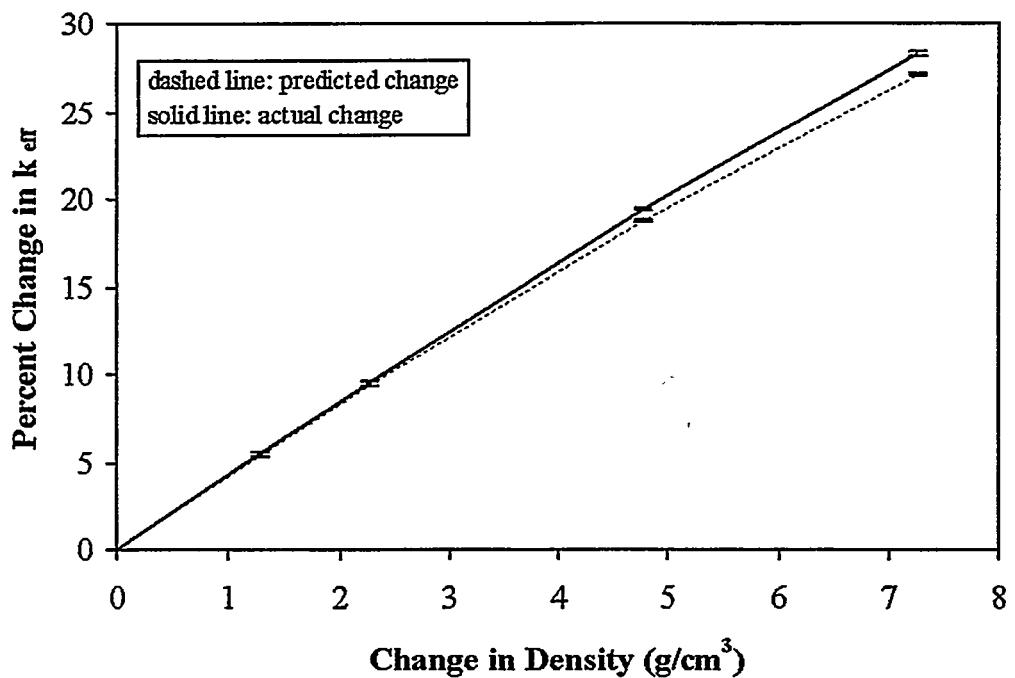


Fig. 1. Godiva-Density Perturbation. Plotted results were calculated by MCNP4C.

## B. Godiva-Composition Change

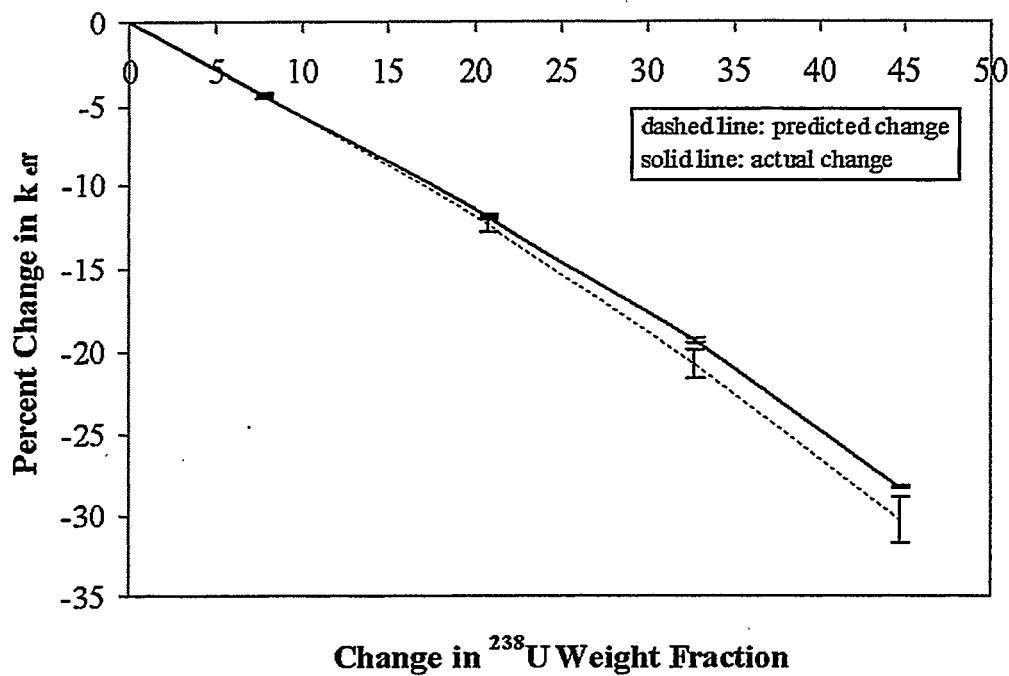
In the KCODE problem “gonc1”, the composition of the Godiva critical assembly was perturbed from its original 94.73%  $^{235}\text{U}$  and 5.27%  $^{238}\text{U}$  to 50% by weight of each isotope. As in “godival”, a track-length estimate was used to calculate  $k_{\text{eff}}$ , and the unperturbed  $k_{\text{eff}}$  is again  $0.998063 \pm 0.000798$ . Table II gives the results for this problem, and Fig. 2 contains a graph of the MCNP4C results. The second-order perturbation accurately predicts, within statistics, the actual  $k_{\text{eff}}$  estimator up to about 5%, after which a second-order perturbation underestimates. The MCNP4C results were in better agreement with those calculated by Densmore et al. in Ref. 3.

## C. Test Problem INP18- $k_{\text{eff}}$ Estimate

The KCODE problem “inp181” is based upon problem INP18 from the MCNP4B test suite. The geometry is a hexagonal lattice core of a light water reactor. Changes were made to the input file to perturb the density of the fuel from  $13.75 \text{ g/cm}^3$  to  $26 \text{ g/cm}^3$ . Again, a track-estimate of  $k_{\text{eff}}$  was calculated using an F4 card and an appropriate tally multiplier. The unperturbed value for  $k_{\text{eff}}$  was found to be  $1.05046 \pm 0.00116$ . The MCNP4C results are presented in Table III and in Fig. 3. The MCNP4C cross-section-dependent perturbed tallies were found to match those of Densmore et al. for the 5% tally perturbation. However, above 5%, MCNP4C was found to better estimate the actual response than Ref. 3.

**TABLE II: Godiva Composition Perturbation —  $k_{\text{eff}}$  Estimate**

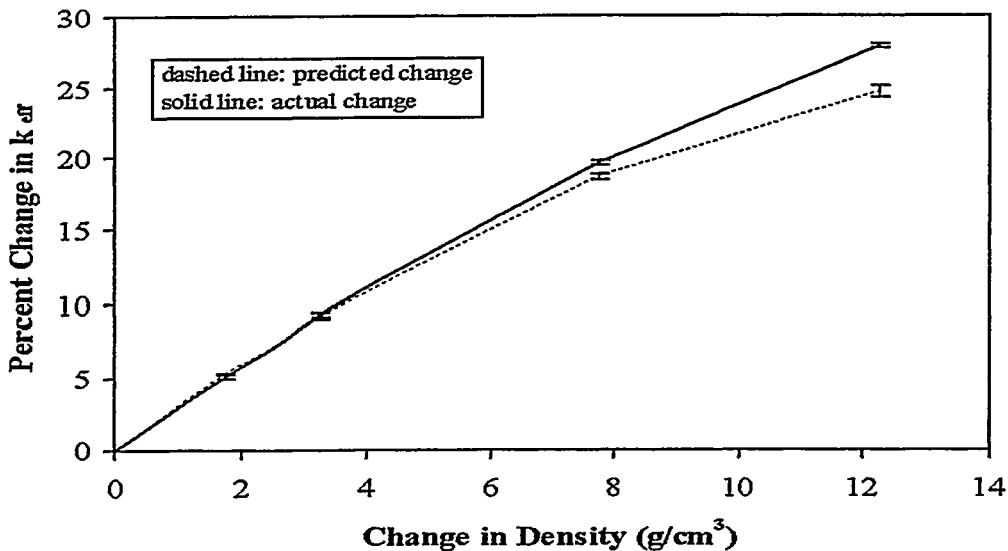
U-238 Weight Fraction (%)	MCNP4C Percent Change (Predicted)	MCNP4C Standard Deviation	Ref.3 Percent Change (Predicted)	Ref. 3 Standard Deviation	Percent Change (Actual)	Standard Deviation (Actual)
13	-4.233	0.084	-4.307	0.082	-4.251	0.111
26	-12.292	0.357	-12.89	0.33	-11.749	0.107
38	-20.778	0.796	-22.31	0.74	-19.346	0.104
50	-30.269	1.423	-33.2	1.3	-28.273	0.101



**Fig. 2. Godiva-Composition Perturbation.** Plotted results were calculated by MCNP4C.

**TABLE III: Test Problem INP18 —  $k_{\text{eff}}$  Estimate**

Density (g/cm <sup>3</sup> )	MCNP4C Percent Change (Predicted)	MCNP4C Standard Deviation	Ref.3 Percent Change (Predicted)	Ref. 3 Standard Deviation	Percent Change (Actual)	Standard Deviation (Actual)
15.5	5.417	0.044	4.970	0.047	5.212	0.152
17	9.128	0.078	8.735	0.084	9.307	0.155
21.5	18.690	0.203	17.30	0.23	19.622	0.164
26	24.680	0.386	21.78	0.50	27.868	0.162



**Fig. 3. Test Problem INP18- $k_{\text{eff}}$  Estimate. Plotted results were calculated by MCNP4C.**

Again, the second-order perturbation is useful up to about 5%. Notice in this problem that the discrepancy between the actual and predicted values increases at a greater rate as density is increased rather than in the Godiva examples. This difference is due to the fact that eigenfunctions are more easily perturbed by density and composition changes in reflected thermal systems than in bare fast system.

#### D. Test Problem INP02-Neutron Absorption Rate Estimate

The fixed-source problem “inp021” is based upon problem INP02 from the MCNP4B test suite. The geometry is a large set of spheres with an inner region of boron surrounded by an aluminum shell. Within this aluminum shell is another set of spheres filled with aluminum. A neutron source is distributed in the boron sphere and has a uniform energy spectrum of 0.1 to 10 MeV. A density perturbation is performed upon the innermost aluminum sphere from 2.7 g/cm<sup>3</sup> to 3.6 g/cm<sup>3</sup>. Using an F4 tally and an appropriate tally multiplier card, the neutron absorption rate is calculated. The unperturbed tally was found to be  $(6.58286 \pm 0.1125) \times 10^{-8}$ . The results from this problem are given in Table IV and in Fig. 4.

TABLE IV: Test Problem INP02 — Neutron Absorption Rate Estimate

Density (g/cm <sup>3</sup> )	MCNP4C Percent Change (Predicted)	MCNP4C Standard Deviation	Ref.3 Percent Change (Predicted)	Ref. 3 Standard Deviation	Percent Change (Actual)	Standard Deviation (Actual)
2.85	5.620	0.142	5.61	0.14	5.629	2.460
3	11.247	0.286	11.25	0.28	11.139	2.534
3.3	22.521	0.578	22.52	0.56	22.044	2.682
3.6	33.823	0.875	33.82	0.83	33.410	2.895

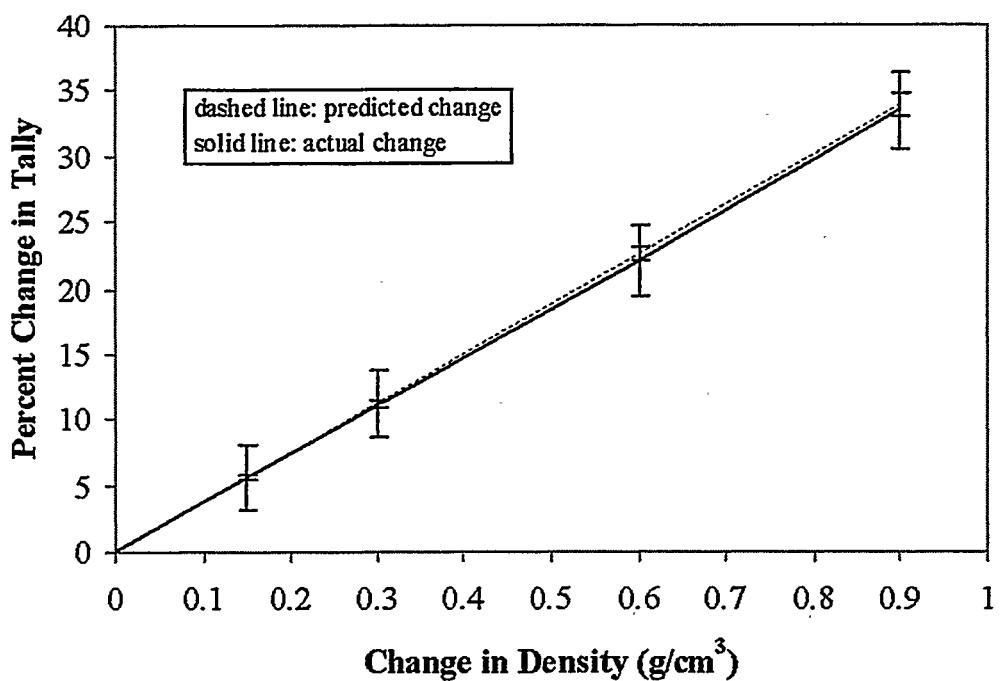


Fig. 4. Test Problem INP02—Neutron Absorption Rate Estimate. Plotted results were calculated by MCNP4C.

As can be seen, the second-order perturbation predicts, within statistics, the actual MCNP tally up to at least a 30% increase in the unperturbed tally. Although the large error in the actual

tally indicates that more histories should have been run, the corrected perturbation still predicts the tally well. MCNP4C results also match those calculated by Densmore et al. within statistics.

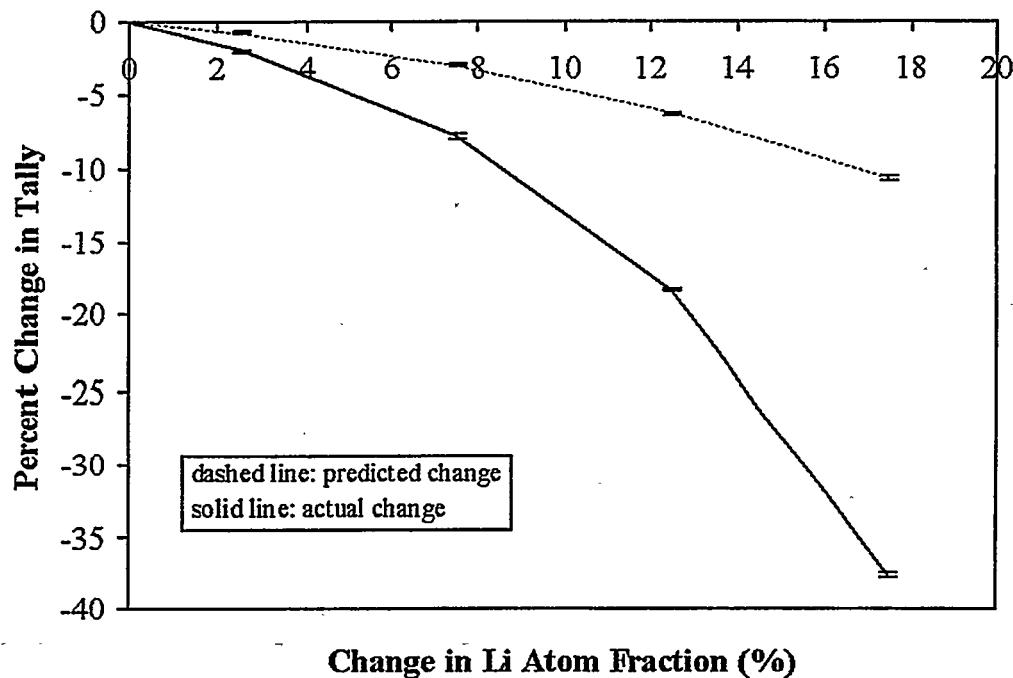
### E. Test Problem INP04—Photon Collision Rate Estimate

This fixed-source problem “inp041” is based upon problem INP04 from the MCNP4B test suite. In this geometry there is a large inner sphere composed of  $\text{UH}_3$  with an outer shell of  $\text{ULi}_3$ . This sphere contains two smaller spheres of  $\text{ULi}_3$ . A 3 MeV photon point source is placed in the center of the large sphere, and the photon collision rate is calculated in the outer shell via an F4 tally with an appropriate tally multiplier card. A composition perturbation was established from 75% Lithium, 25% Uranium to 92.5% Lithium, 7.5% Uranium where the percents are given in atom percent. The unperturbed tally for this problem was found to be  $(6.98722 \pm 0.00629)\text{E-4}$ . The results from this problem are given in Table V and in Fig. 5.

TABLE V: Test Problem INP04 — Photon Collision Rate Estimate

Li Atom Fraction (%)	MCNP4C Percent Change (Predicted)	MCNP4C Standard Deviation	Ref.3 Percent Change (Predicted)	Ref. 3 Standard Deviation	Percent Change (Actual)	Standard Deviation (Actual)
77.5	-0.734	0.016	-0.726	0.022	-1.975	0.126
82.5	-2.993	0.056	-2.921	0.083	-7.852	0.123
87.5	-6.306	0.112	-6.11	0.17	-18.348	0.117
92.5	-10.672	0.183	-10.28	0.34	-37.598	0.115

In Table V, a quick comparison between MCNP4C values and those of Densmore et al. shows that these tally results match within statistics. However, as can be seen in Fig. 5, the corrected perturbation does not predict the actual values very well. As explained in Ref. 3, the reason is that the second-order perturbation is on the order of fifteen percent the total perturbation for the 5% tally perturbation. The total and first-order perturbations are shown in Table VI. In the 5% tally perturbation case, the limitations of only using the first two Taylor series expansions in the differential operator technique start to show. This approximation can only be made more accurate if more terms are used in the expansion.



**Fig. 5. Test Problem INP04—Photon Collision Rate Estimate. Plotted results were calculated by MCNP4C.**

**TABLE VI: Lithium Bin Uncorrected Perturbations**

Li Atom Fraction (%)	First-Order Corrected Perturbation	Total Corrected Perturbation
77.5	-4.2119E-6	-5.1049E-6
92.5	-2.9483E-5	-7.3238E-5

The situation is worse for the 30% increase in the unperturbed tally (92.5% Li). For this perturbation the second-order term is almost equal to that of the first-order term. This problem demonstrates that the perturbation feature cannot accurately predict every tally, and a second-order Taylor series approximation will fail if the tally exhibits higher than second-order behavior.

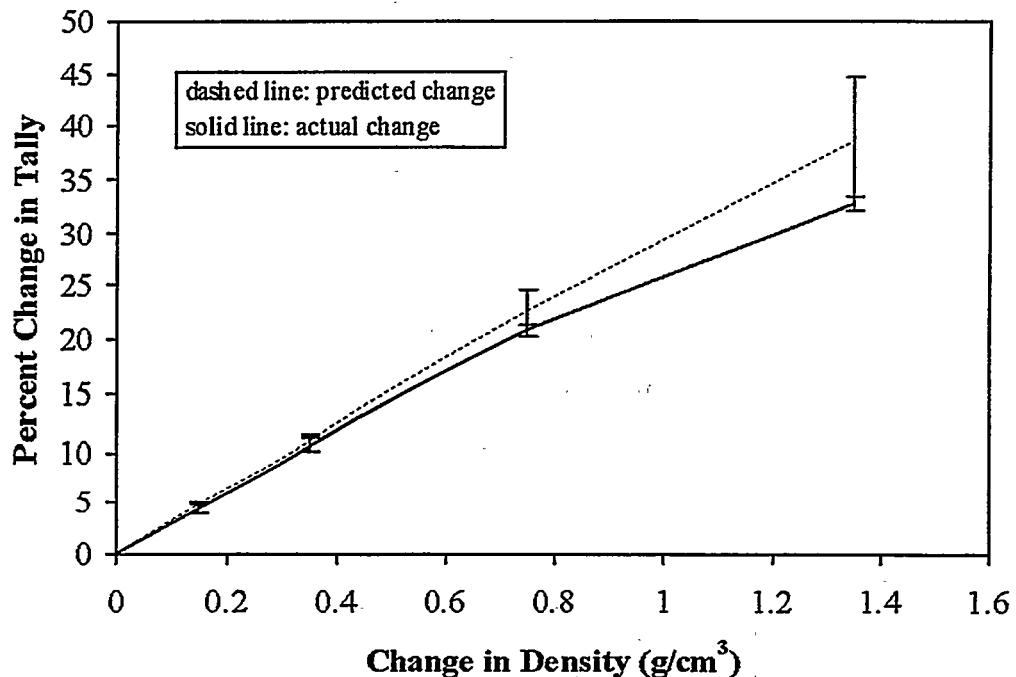
## F. Test Problem INP10—Photon Collision Rate Estimate

This fixed-source problem “inp101” is based upon problem INP10 from the MCNP4B test suit. The geometry of this problem consists of two concentric infinite cylinders. The inner cylinder is filled with water, and the outer shell is filled with copper. Near the origin the inner cylindrical region is separated into several disks filled with water or carbon and one that is void.

The void disk contains a cube of CuO, and an adjacent disk of water contains a void torus surrounded by a shell of copper. A Watt fission spectrum neutron source is distributed evenly in the CuO cube, and the photon collision rate is tallied in one of the carbon disks via an F4 tally with an appropriate multiplier card. A density perturbation was established from 2.25 g/cm<sup>3</sup> to 3.6 g/cm<sup>3</sup> in the carbon disk. The unperturbed tally was found to be (6.63928±0.02324)E-6. The results from this problem are given in Table VII and in Fig. 6.

**TABLE VII: Test Problem INP10 — Photon Collision Rate Estimate**

Density (g/cm <sup>3</sup> )	MCNP4C Percent Change (Predicted)	MCNP4C Standard Deviation	Ref.3 Percent Change (Predicted)	Ref. 3 Standard Deviation	Percent Change (Actual)	Standard Deviation (Actual)
2.4	4.799	0.146	4.80	0.14	4.492	0.499
2.6	11.007	0.502	11.01	0.48	10.673	0.515
3	22.768	1.946	22.8	1.9	20.827	0.545
3.6	38.770	6.011	38.8	5.9	32.822	0.573



**Fig. 6. Test Problem INP10–Photon Collision Rate Estimate. Plotted results were calculated by MCNP4C.**

Again, the MCNP4C predicted perturbations matched those of Densmore et al. within statistics. Also, the second-order corrected perturbation predicts the actual MCNP values well up to a 30% increase in the unperturbed tally. Although the perturbation begins to diverge from the actual value after about a 10% increase in the unperturbed tally, the predicted values agree with the actual values, within statistics, up to 30%. The high standard deviations could be reduced by using more particle histories in the estimate.

## VI. PERTURBATION CONVERGENCE

Further tests were run to verify that a perturbation converges to the expected value. Several pairs of problems were created to be used for these tests and were named the “fm7#” test set. The perturbation was substituted for what it was perturbing in the “fm7#b” test set. In this way, for long runs on “fm7#” problems, an agreeing tally (and agreeing estimate of  $k_{\text{eff}}$  where appropriate) was expected in the corresponding “fm7#b” problem. The following sections detail the convergence test tally results and references to  $k_{\text{eff}}$  refer to the final estimated combined collision/absorption/track-length  $k_{\text{eff}}$ . The input files are included in Appendix A, Section H.

### A. Neutron Density Perturbation Problem

In problem fm73, a density perturbation in cell 1 was established in a KCODE problem using the following cards:

Cell card: 1 1 0.0479813 -1

Perturbation card: PERT1:n CELL=1 RHO=0.054 METHOD=1

Perturbation card: PERT2:n CELL=1 RHO=0.054 METHOD=3 .

Then problem fm73b was created with the density on the cell card changed to 0.054, and both PERT cards deleted. Results from both runs were as follows:

Tally from fm73b:	1.08219E0	Rel. Err.	0.0001
Tally from fm73:	9.98070E-1	Rel. Err.	0.0001
PERT1 tally from fm73:	8.06083E-2	Rel Err.	0.0004
PERT2 tally from fm73:	-2.78845E-3	Rel. Err.	0.0017
$k_{\text{eff}}$ from fm73:	0.99804	Rel. Err.	0.00012
$k_{\text{eff}}$ from fm73b:	1.07822	Rel. Err.	0.00013
PERT1 to $k_{\text{eff}}$ from fm73:	0.08062	Rel. Err.	0.00004
PERT2 to $k_{\text{eff}}$ from fm73:	-0.00278	Rel. Err.	0.00000

Since the second-order Taylor series term is less than 20% the total perturbation, then one can assume that this perturbation can be well approximated using only the first two expansion terms. Thus, the actual percent change of the tally was 8.4%, and the predicted with the PERT card was 8.6%. The actual percent change of  $k_{\text{eff}}$  was 8.03%, and the predicted change was 8.08%.

## B. Neutron Material Perturbation Problem

In the KCODE problem fm71, a material perturbation in cell 1 was established using the following cards:

Material card:m1 92235 -94.73 92238 -5.27

Material card:m2 92235 -87 92238 -13

Tally Multiplier Card:-1 1 -6 -7:-2

Perturbation card: PERT1:n CELL=1 MAT=2 METHOD=-1 RXN= -6 -2

Perturbation card: PERT2:n CELL=1 MAT=2 METHOD=3 RXN= -6 -2

Then problem fm71b was created by deleting the material 1 card, renaming material 2 as material 1, and deleting the PERT cards. Results from both runs were as follows:

Tally from fm71b:	1.000194E0	Rel. Err.	0.0001
Tally from fm71:	1.041530E0	Rel. Err.	0.0001
PERT1 tally from fm71:	9.99553E-1	Rel Err.	0.0001
PERT2 tally from fm71:	-1.58480E-3	Rel Err.	0.0003
$k_{\text{eff}}$ from fm71b:	0.95404	Rel. Err.	0.00012
$k_{\text{eff}}$ from fm71:	0.99731	Rel. Err.	0.00012
PERT1 to $k_{\text{eff}}$ from fm71:	0.95396	Rel. Err.	0.00012
PERT2 to $k_{\text{eff}}$ from fm71:	-0.00150	Rel. Err.	0.00000

Since the second-order Taylor series term is less than 20% the total perturbation, then one can assume that this perturbation can be well approximated using only the first two expansion terms. The actual percent change of the tally was 3.97%, and the predicted percent change was 4.03%. The actual percent change of  $k_{\text{eff}}$  was 4.34%, and the predicted change was 4.35%.

## C. Photon Density Perturbation Problem with Nonsequentially Numbered Cells

In photon problem fm72, a density perturbation in cells 1 and 4 was established using the following cards:

Cell card:1 1 0.0479813 -1

Cell card:4 1 0.0479813 -23 (215 : 216 : -217)

Tally card:f4:p 1

Tally card:f24:p 4

Tally Multiplier Card:fm4 -1 1 -4 :-3

Tally Multiplier Card:fm24 -1 1 2 :-4 :-3

Perturbation card: PERT1:p CELL=1 METHOD=-1 RHO=0.0485 RXN=-4 -3

Perturbation card: PERT2:p CELL=1 METHOD=-2 RHO=0.0485 RXN=-4 -3

Perturbation card: PERT3:p CELL=4 METHOD=-1 RHO=0.0485 RXN=-4 -3 -2

Then problem fm72b was created with the density on the material cards replaced with 0.0485, and the PERT cards deleted. Results from both runs were as follows:

Tally 4 from fm72b:	2.22759E1	Rel. Err.	0.0024
Tally 4 from fm72:	2.21429E1	Rel. Err.	0.0024
PERT1 on tally 4 from fm72:	2.22871E1	Rel Err.	0.0024
PERT2 on tally 4 from fm72:	2.22833E1	Rel Err.	0.0024
Tally 24 from fm72b:	4.53982E0	Rel. Err.	0.0075
Tally 24 from fm72:	4.43319E0	Rel. Err.	0.0074
PERT3 on tally 24 from fm72:	4.56925E0	Rel Err.	0.0074

Again, the second-order Taylor series term is less than 20% the total perturbation. The actual percent change of tally 4 was 0.60%, and the predicted percent change was 0.65%. The actual percent change of tally 24 was 2.3%, and the predicted percent change was 3.0% which is within the 0.74% relative error.

#### D. Neutron KCODE Density and Repeated Nuclide Perturbation Problem

In problem fm75, material and density perturbations in cell 1 were established using the following cards:

Cell card:1 0.0479813 -1

Material card:m1 92235.50c 0.5 92238.50c 0.5

Material card:m2 92235.50c 0.1 92235.50c 0.4 92238.50c 0.5

Tally Card:f4:n 1

Tally Multiplier Card:fm4 -1 1 1

Perturbation card: PERT1:n CELL=1 MAT=1 RHO=0.05 METHOD=1

Perturbation card: PERT2:n CELL=1 MAT=1 RHO=0.05 METHOD=2

Perturbation card: PERT3:n CELL=1 MAT=2 RHO=0.05 METHOD=1

Perturbation card: PERT4:n CELL=1 MAT=2 RHO=0.05 METHOD=2

Then problem fm75b was created with the material 1 card information replaced by material 2 information, the density on the cell 1 card switched to 0.05, and the PERT cards deleted. Since both material compositions are the same, it is expected that the perturbed tallies should match (pert1 and pert2 on tally4). Results from both runs were as follows:

Tally from fm75b:	3.31448E0	Rel. Err.	0.0001
Tally from fm75:	3.17270E0	Rel. Err.	0.0001
PERT1 tally from fm75:	1.37281E-1	Rel Err.	0.0005
PERT2 tally from fm75:	1.37374E-1	Rel Err.	0.0004
PERT3 tally from fm75:	1.37281E-1	Rel Err.	0.0005
PERT4 tally from fm75:	1.37374E-1	Rel Err.	0.0004
$k_{eff}$ from fm75:	0.72238	Rel. Err.	0.00009
$k_{eff}$ from fm75b:	0.75037	Rel. Err.	0.0001
PERT1 to $k_{eff}$ from fm75:	0.02790	Rel. Err.	0.00001
PERT2 to $k_{eff}$ from fm75:	0.02810	Rel. Err.	0.00001
PERT3 to $k_{eff}$ from fm75:	0.02790	Rel. Err.	0.00001
PERT4 to $k_{eff}$ from fm75:	0.02810	Rel. Err.	0.00001

The second-order Taylor series term is less than 20% the total perturbation. The actual percent change of the tally was 4.3%, and the predicted percent change was 4.1%. The actual percent change of  $k_{eff}$  was 3.87%, and the predicted change was 3.86%.

## VII. UPGRADE OF INSTALLATION TEST SUITE

Due to addition of the cross-section dependent perturbed tally feature to MCNP4C, the version 4B installation test suite required upgrading. This new feature is now tested during MCNP compilation. Several features of the previously described test problems were combined with the 4B installation test suite files. The new test suite problems extend the installation tests across the new cross-section dependent tally perturbation capability. These problems include tests on all previously found perturbation errors including: RXN=-1 for neutrons, RXN=-5 for photons, repeated nuclides, and RXN specifications on a combined particle PERT card.

Three suite problems have been altered and are included in Appendix E. These additions slowed the test problems: inp10 by 4%, inp11 by 1%, and inp18 by 5%. The following sections give a brief description of the changes and reasons for them.

#### **A. Changes to Suite Problem Inp10**

Additions and changes made to test problem inp10 include:

- adding a material 5 so that a material perturbation could be tested;
- adding FM cards for the two tallies so that the negative multiplicative constant could be used to turn on the cross-section dependent tally capability;
- adding two SD cards to divide the tallies by the cell volumes;
- and adding five material and/or density perturbations used to test differing RXN and FM reaction numbers for neutrons or photons.

#### **B. Changes to Suite Problem Inp11**

Additions and changes made to test problem inp11 include:

- adding a fourth neutron tally (named 34) on cell 2;
- adding one SD card for the new tally;
- adding one FM card for the new tally which matches the FM card for tally 14 except uses negative multiplicative constants;
- adding two new perturbations; one for testing the fatal error expected with a mixed particle perturbation and the RXN specified (the runprob used during installation uses the fatal option on the command line for this problem); the second for neutron perturbation which tests a list of reactions.

#### **C. Changes to Suite Problem Inp18**

Additions and changes made to test problem inp18 include:

- repeating the tally, comment, and segment divisor from tally 4 but renaming them 14;
- repeating the FM card for tally4 but renaming it to 14 and changing the multiplicative constants to negative values to turn on the perturbation correction feature.

## VIII. SUMMARY

Implementation of the cross-section dependent tally feature into MCNP4C has been completed. This capability will appropriately add a term to the calculated perturbation for type 6 and type 7 tallies and type 4 tallies with FM cards using a negative multiplicative constant.

Verification of capability correctness has been completed using various input files created specifically to test relative parameters and options. The results presented in this report verify the applicability and correctness of many perturbation features including the new cross-section dependent tally feature. These tests included comparisons of converged perturbed results to converged results of an identical problem using the perturbed parameters. The installation test suite problems have been updated to test the new capability during MCNP4C installation.

## REFERENCES

1. J. Briesmeister, Editor, "MCNP<sup>TM</sup>—A General Monte Carlo N-Particle Transport Code: Version 4B," LA-12625-M, Version 4B, Los Alamos National Laboratory (1997).
2. G. W. McKinney and J. L. Iverson, "Verification of the Monte Carlo Differential Operator Technique for MCNP<sup>TM</sup>," LA-13098, Los Alamos National Laboratory, (1996).
3. J. D. Densmore, G. W. McKinney, and J. S. Hendricks, "Correction to the MCNP<sup>TM</sup> Perturbation Feature for Cross-Section Dependent Tallies," LA-13374, Los Alamos National Laboratory, (1997).
4. G. W. McKinney, "Theory Related to the Differential Operator Perturbation Technique," Los Alamos National Laboratory Memo, X-6:GWM-94-124 (1994).
5. J. S. Hendricks, "Proposed MCNP4C Manual Revisions," Los Alamos National Laboratory Memo, XCI:JSH-98-99 (U) - rev. 1 (1998).

## APPENDIX A

### MCNP VERIFICATION TEST FILES

#### I. OVERVIEW

Included here are the test files used to verify the perturbation feature with the cross-section dependent tally capability. Most files were based upon a Godiva density- or composition-perturbation problem found on pages 29 and 30 of LA-13374.<sup>3</sup> Since the purpose of these tests was to ensure option correctness, a standard perturbation was used and the option parameters were varied. Due to redundancies in input files, several problems are presented as alterations to previously shown files.

#### II. TEST INPUT FILES

The sections presented here include the input files which were used to check for MCNP4C cross-section dependent tally feature correctness. The subsections are titled after the sections in the main document for which the input files correspond. The expected results of each file are discussed here unless noted otherwise.

##### A. Validation of MT Versus FM Reaction Numbers

These files were created to test the MT versus FM reaction numbers on the RXN parameter of the PERT card.

**1. Input File Mtfm01.** This input file compares expected values using the default (pert1), MT (pert2), FM (pert3), total reaction numbers and a blank RXN card (pert4) in a neutron problem. All perturbations should match.

Godiva problem in LA-13374 on pg 30 used to compare MT to FM reactions

```
1 1 0.0479813 -1
2 0 1
```

```
1 so 8.741
```

```
kcode 1000 1.0 10 40
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
m2 92235.50c -87 92238.50c -13
f4:n 1
```

```
f14:n 1
fm4 -1 1 1
fm14 -1 1 -1
sd4 1
sd14 1
pert1:n cell=1 rho=-18.74 mat=2 method=-1
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=1
pert3:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-1
pert4:n cell=1 rho=-18.74 mat=2 method=-1 rxn=
prdmp 2j -1
```

**2. Input File Mtfm02.** This input file compares expected values using the MT (pert3), FM (pert2) neutron absorption reaction numbers and the equivalent sum of reactions 102 through 107 (pert1). All perturbations on corresponding FM cards should match (pert1 on tally4, pert2 on tally 14, and pert 3 on tally 24).

Replace tally section in mtfm01 (lines 12 through 17) with:

```
f4:n 1
f14:n 1
f24:n 1
fm4 -1 1 102:103:104:105:106:107
fm14 -1 1 -2
fm14 -1 1 101
sd4 1
sd14 1
sd24 1
```

Replace mtfm01 perturbation lines (18 through 21) with:

```
pert1:n cell=1 rho=-18.74 mat=2 method=-1 rxn=102 103 104 105 106 107
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-2
pert3:n cell=1 rho=-18.74 mat=2 method=-1 rxn=101
```

**3. Input File Mtfm03.** This input file compares expected values using the MT (pert1) and FM (pert2) neutron elastic scattering reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm01 (lines 14 through 15) with:

```
fm4 -1 1 2
fm14 -1 1 -3
```

Replace mtfm01 perturbation lines (18 through 21) with:

```
pert1:n cell=1 rho=-18.74 mat=2 method=-1 rxn=2
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-3
```

**4. Input File Mtfm06.** This input file compares expected values using the MT (pert1) and FM (pert2) neutron total fission reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm01 (lines 14 through 15) with:

```
fm4 -1 1 19:20:21:38
fm14 -1 1 -6
```

Replace mtfm01 perturbation lines (18 through 21) with:

```
pert1:n cell=1 rho=-18.74 mat=2 method=-1 rxn=19 20 21 38
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-6
```

**5. Input File Mtfm31.** This input file compares expected values using the MT (pert1) and FM (pert2) photon incoherent scattering reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Godiva problem in LA-13374 on pg 30 used to compare MT to FM reactions

```
1 1 0.0479813 -1
```

```
2 0 1
```

```
1 so 8.741
```

```
mode p
nps 10000
sdef pos 0 0 0
imp:p 1 0
m1 92235 -94.73 92238 -5.27
f4:p 1
f14:p 1
fm4 -1 1 504
fm14 -1 1 -1
sd4 1
sd14 1
pert1:p cell=1 rho=0.045 method=-1 rxn=504
pert2:p cell=1 rho=0.045 method=-1 rxn=-1
prdmp 2j -1
```

**6. Input File Mtfm32.** This input file compares expected values using the MT (pert1) and FM (pert2) photon coherent scattering reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm31 (lines 14 through 15) with:

```
fm4 -1 1 502
fm14 -1 1 -2
```

Replace mtfm31 perturbation lines (18 through 19) with:

```
pert1:p cell=1 rho=0.045 method=-1 rxn=502
pert2:p cell=1 rho=0.045 method=-1 rxn=-2
```

**7. Input File Mtfm33.** This input file compares expected values using the MT (pert1) and FM (pert2) photon photoelectric reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm31 (lines 14 through 15) with:

```
fm4 -1 1 522
fm14 -1 1 -3
```

Replace mtfm31 perturbation lines (18 through 19) with:

```
pert1:p cell=1 rho=0.045 method=-1 rxn=522
pert2:p cell=1 rho=0.045 method=-1 rxn=-3
```

**8. Input File Mtfm34.** This input file compares expected values using the MT (pert1) and FM (pert2) photon pair production reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm31 (lines 14 through 15) with:

```
fm4 -1 1 516
fm14 -1 1 -4
```

Replace mtfm31 perturbation lines (18 through 19) with:

```
pert1:p cell=1 rho=0.045 method=-1 rxn=516
pert2:p cell=1 rho=0.045 method=-1 rxn=-4
```

**9. Input File Mtfm35.** This input file compares expected values using the default (pert1), MT (pert2), FM (pert3), total reaction numbers, and a blank RXN card (pert4) in a photon problem. All perturbations should match.

Replace tally FM card section in mtfm31 (lines 14 through 15) with:

```
fm4 -1 1 501
fm14 -1 1 -5
```

Replace mtfm31 perturbation lines (18 through 19) with:

```
pert1:p cell=1 rho=0.045 method=-1
pert2:p cell=1 rho=0.045 method=-1 rxn=501
pert3:p cell=1 rho=0.045 method=-1 rxn=-5
pert4:p cell=1 rho=0.045 method=-1 rxn=
```

**10. Input File Mtfm81.** This input file compares expected values using the default (pert1), MT (pert2), FM (pert3), total reaction numbers, and a blank RXN card (pert4) in a multi-group neutron problem. All perturbations should match down to the last decimal place where they are different. This is due to the total edit cross section (MT=1) not being equal to the transport cross section (MT=-1). The cross-section data only match up to the first five digits of the value. This creates a discrepancy in the final calculated data.

Godiva problem in LA-13374 on pg 30 checking FM and MT perturbation reactions

```
1 1 0.0479813 -1
2 0 1
```

```
1 so 8.741
```

```
kcode 1000 1.0 10 40
```

```

ksrc 0 0 0
imp:n 1 0
m1 92235 -94.73 92238 -5.27
m2 92235 -87 92238 -13
mode n
mgopt f 30
f4:n 1
f14:n 1
fm4 -1 1 1
fm14 -1 1 -1
sd4 1
sd14 1
pert1:n cell=1 rho=-18.74 mat=2 method=-1
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=1
pert3:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-1
pert4:n cell=1 rho=-18.74 mat=2 method=-1 rxn=
prdmp 2j -1

```

**11. Input File Mtfm82.** This input file compares expected values using the MT (pert1) and FM (pert2) multigroup neutron fission reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm81 (lines 16 through 17) with:

```

fm4 -1 1 18
fm14 -1 1 -2

```

Replace mtfm81 perturbation lines (20 through 23) with:

```

pert1:n cell=1 rho=-18.74 mat=2 method=-1 rxn=18
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-2

```

**12. Input File Mtfm83.** This input file compares expected values using the MT (pert1) and FM (pert2) multigroup neutron absorption reaction numbers on the RXN parameter. All perturbations on corresponding FM cards should match (pert1 on tally4 and pert2 on tally 14).

Replace tally FM card section in mtfm81 (lines 16 through 17) with:

```

fm4 -1 1 101
fm14 -1 1 -5

```

Replace mtfm81 perturbation lines (20 through 23) with:

```

pert1:n cell=1 rho=-18.74 mat=2 method=-1 rxn=101
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=-5

```

## B. Reaction List on RXN Parameter

The following sections detail the input files and their expected results. These files were created to test the perturbation RXN parameter when using a list of reactions rather than a single reaction.

**1. Input File Lis01.** This neutron problem is based on a density perturbation. The reaction list includes MT numbers which correspond to the total fission cross section. The two unperturbed tallies are expected to match each other as should the two perturbed tallies.

problem used to check rxn list

```
1 1 0.0479813 -1
2 0 1
```

```
1 so 8.741
```

```
sdef erg=d1 pos=0 0 0
```

```
si1 1 14
```

```
sp1 0 1
```

```
nps 1000
```

```
imp:n 1 0
```

```
m1 92238 1
```

```
f4:n 1
```

```
fm4 -1 1 -6
```

```
sd4 1
```

```
f14:n 1
```

```
fm14 -1 1 19:20:21:38
```

```
sd14 1
```

```
pert1:n cell=1 rho=0.047 method=-1 rxn=-6
```

```
pert2:n cell=1 rho=0.047 method=-1 rxn=19 20 21 38
```

```
prdmp 2j -1
```

**2. Input File Lis31.** This photon problem is based on a density perturbation. The reaction list includes MT numbers which correspond to the total cross section. The two unperturbed tallies are expected to match each other as should the two perturbed tallies (pert1 on tally 4 and pert2 on tally14).

Problem used to check reaction lists

```
1 1 0.0479813 -1
```

```
2 0 1
```

```
1 so 8.741
```

```
mode p
```

```
nps 1000
```

```
sdef pos 0 0 0
```

```
imp:p 1 0
```

```
m1 92235 -94.73 92238 -5.27
```

```
f4:p 1
```

```
f14:p 1
```

```
fm4 -1 1 -1:-2:-3:-4
```

```
fm14 -1 1 -5
```

```
sd4 1
```

```
sd14 1
```

```
pert1:p cell=1 rho=0.048 method=-1 rxn=-1 -2 -3 -4
```

```
pert2:p cell=1 rho=0.048 method=-1 rxn=-5
```

```
prdmp 2j -1
```

### C. Nonsequentially Numbered Cells

This section describes the input files used to ensure that nonsequentially numbered cells did not deter the perturbation feature from operating correct. For each test, a pair of files was created. The first file contains the perturbations and nonsequentially numbered cells. The second file contains all perturbations but uses sequentially numbered cells.

**1. Input File Mis01.** This neutron input file was generated to be certain that the changes to the perturbation feature could deal with MCNP's internal referencing which must be done when cells are not numbered in order. Three tallies are established: one on the inner sphere, one on the box cell excluding the sphere, and another on the area outside the box cell but inside the outer sphere. Unperturbed and perturbed tally results should match those of mis01b.

Altered Godiva problem in LA-13374 on pg 30 used to check for perturbations on  
c non-sequentially numbered cell cards

```
1 1 0.0479813 -1
15 1 0.0479813 1 -215 -216 217
4 1 0.0479813 -23 (215: 216 : -217)
37 0 23
```

```
1 so 2
215 cx 3
216 px 5
217 px -4
23 so 8
```

```
kcode 1000 1.0 20 500
ksrc 0 0 0
imp:n 1 1 1 0
m1 92235 -94.73 92238 -5.27
m2 92235 -87 92238 -13
f4:n 1
f14:n 15
f24:n 4
fm4 -1 1 -6 -7
fm14 -1 1 -6 -7
fm24 -1 1 -6 -7
sd4 1
sd14 1
sd24 1
pert1:n cell=1 mat=2 method=1 rxn= -6
pert2:n cell=1 mat=2 method=2 rxn= -6
pert3:n cell=1 mat=2 method=3 rxn= -6
pert4:n cell=4 mat=2 method=-1 rxn= -6
prdmp 2j -1
dbcn
```

**2. Input File Mis01b.** This input file was generated starting with mis01 but renumbering the cells and surfaces to be sequentially numbered. Unperturbed and perturbed tally results should match those of mis01.

Replace the cell and surface definitions of mis01 (lines 1-10) with:

```
1 1 0.0479813 -1
2 1 0.0479813 -2 (3:4:-5)
3 1 0.0479813 1 -3 -4 5
4 0 2
```

```
1 so 2
2 so 8
3 cx 3
4 px 5
5 px -4
```

Replace the tally definitions of mis01 (lines 17-19) with:

```
f4:n 1
f14:n 3
f24:n 2
```

Replace the perturbation definitions of mis01 (lines 26-29) with:

```
pert1:n cell=1 mat=2 method=1 rxn= -6
pert2:n cell=1 mat=2 method=2 rxn= -6
pert3:n cell=1 mat=2 method=3 rxn= -6
pert4:n cell=2 mat=2 method=-1 rxn= -6
```

**3. Input File Mis31.** This photon input file was also generated to be certain that the changes to the perturbation feature could deal with MCNP's internal referencing which must be done when cells are not numbered in order. This problem is essentially the same as mis01 except this one uses a source definition to generate photons. Three tallies are established: one on the inner sphere, one on the box cell excluding the sphere, and another on the area outside the box cell but inside the outer sphere. Unperturbed and perturbed tally results should match those of mis31b.

Photon problem used to check for non-sequentially numbered cell cards and the perturbation feature

```
1 1 0.0479813 -1
15 1 0.0479813 1 -215 -216 217
4 1 0.0479813 -23 (215:216:-217)
37 0 23
```

```
1 so 2
215 cx 3
216 px 5
217 px -4
23 so 8
```

nps 10000

```

mode p
sdef pos 0 0 0
imp:p 1 1 1 0
m1 92235 -94.73 92238 -5.27
f4:p 1
f14:p 15
f24:p 4
fm4 -1 1 -5
fm14 -1 1 -5
fm24 -1 1 -5
sd4 1
sd14 1
sd24 1
pert1:p cell=1 method=1 rxn= -5 rho=0.048
pert2:p cell=1 method=2 rxn= -5 rho=0.048
pert3:p cell=1 method=3 rxn= -5 rho=0.048
pert4:p cell=4 method=-1 rxn= -5 rho=0.048
prdmp 2j -1
dbcn

```

**4. Input File Mis31b.** This input file was generated starting with mis31 but renumbering the cells and surfaces to be sequentially numbered. Unperturbed and perturbed tally results should match those of mis31.

Photon problem used to check for non-sequentially numbered cell cards and perturbation feature

```

1 1 0.0479813 -1
2 1 0.0479813 -2 (3: 4 : -5)
3 1 0.0479813 1 -3 -4 5
4 0 2

```

```

1 so 2
2 so 8
3 cx 3
4 px 5
5 px -4

nps 10000
mode p
sdef pos 0 0 0
imp:p 1 1 1 0
m1 92235 -94.73 92238 -5.27
f4:p 1
f14:p 3
f24:p 2
fm4 -1 1 -5
fm14 -1 1 -5
fm24 -1 1 -5
sd4 1
sd14 1
sd24 1
pert1:p cell=1 method=1 rxn= -5 rho=0.048
pert2:p cell=1 method=2 rxn= -5 rho=0.048

```

```
pert3:p cell=1 method=3 rxn= -5 rho=0.048
pert4:p cell=2 method=-1 rxn= -5 rho=0.048
prdmp 2j -1
dbcn
```

#### D. Positive and Negative RHO Numbers

The following file tests the use of equivalent positive and negative density specifiers. The two tallies are expected to give identical results.

Godiva problem in LA-13374 on pg 30 used to check response to RHO numbers

```
1 1 0.04 -1
2 0 1
1 so 8.741

kcode 1000 1.0 10 40
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
f4:n 1
fm4 -1 1 1
sd4 1
pert1:n cell=1 rho=-18.7399 method=-1 rxn=1
pert2:n cell=1 rho=0.0479813 method=-1 rxn=1
prdmp 2j -1
```

#### E. Bogus RXN, CELL, MAT, and METHOD Numbers

These files test bogus numbers specified on various parameters of the PERT card. There were no expected results since the response of MCNP4C was being tested. The results were described in the main document. Due to several repetitious definitions, subsequent problems are given as an alteration to the problem given in subsection 1.

**1. Neutron Problem with Photon Reaction on RXN Parameter.** The following input file was used for this test.

Godiva problem in LA-13374 on pg 30 used to check response to bogus rxns

```
1 1 0.0479813 -1
2 0 1
1 so 8.741

kcode 1000 1.0 10 40
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
m2 92235.50c -87 92238.50c -13
f4:n 1
```

```
fm4 -1 1 1
sd4 1
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=501
prdmp 2j -1
```

**2. Unknown Reaction on RXN Parameter.** The following input file was used for this test.

Replace the Perturbation definition (line 15) in the problem of subsection 1 with:  
pert2:n cell=1 rho=-18.74 mat=2 method=-1 rxn=952

**3. Use of Nonexisting Cell on CELL Parameter.** The following input file was used for this test.

Replace the Perturbation definition (line 15) in the problem of subsection 1 with:  
pert2:n cell=3 rho=-18.74 mat=2 method=-1 rxn=1

**4. Use of Nonexisting Material on MAT Parameter.** The following input file was used for this test.

Replace the Perturbation definition (line 15) in the problem of subsection 1 with:  
pert2:n cell=1 rho=-18.74 mat=4 method=-1 rxn=1

**5. Use of Invalid Number on METHOD Parameter.** The following input file was used for this test.

Add the following perturbation to the problem of subsection 1:  
pert2:n cell=1 rho=-18.74 mat=2 method=5 rxn=1

## F. Energy Ranges Via the ERG Parameter

These test files were created to ensure that the new capability still was able to perturb only a range of energies using the ERG parameter of the perturbation feature. The reasoning behind creating these files due to threshold energies is listed in the main document.

**1. Input File Erg01.** This neutron input file was generated with a fixed source and the fission neutrons turned off, so that all neutrons could be expected to be less than the source energy. The unperturbed tallies should be identical, and both perturbed tallies should give identical answers (pert1 on tally4 and pert2 on tally14).

Godiva problem in LA-13374 on pg 30 used to check response to erg option

```
1 1 0.0479813 -1
```

```
2 0 1
```

```
1 so 8.741
```

```
sdef erg=d1 pos=0 0 0
```

```
si1 L 7
sp1 1
nps 1000
nonu
imp:n 1 0
m1 92235.50c 1
f4:n 1
fm4 -1 1 16:17
sd4 1
f14:n 1
fm14 -1 1 16
sd14 1
pert1:n cell=1 rho=0.04 method=1 rxn=16 17 erg=5.5,9
pert2:n cell=1 rho=0.04 method=1 rxn=16 erg=5.5,9
prdmp 2j -1
```

**2. Input File Erg02.** This neutron input file was generated with a fixed source and the fission neutrons turned off, so that all neutrons could be expected to be less than the source energy. For this problem, it is expected that all tallies (unperturbed and perturbed) should match each other.

Godiva problem in LA-13374 on pg 30 used to check response to erg option

```
1 1 0.0479813 -1
2 0 1
```

```
1 so 8.741
```

```
sdef erg=d1 pos=0 0 0
si1 L 5
sp1 1
nps 1000
nonu
imp:n 1 0
m1 92235.50c 1
f4:n 1
fm4 -1 1 -6:-3:16:17
sd4 1
f14:n 1
fm14 -1 1 -6:-3
sd14 1
pert1:n cell=1 rho=0.04 method=-1 rxn=-6 -3 16 17 erg=5.5,9
pert2:n cell=1 rho=0.04 method=-1 rxn=-6 -3 erg=5.5,9
prdmp 2j -1
```

**3. Input File Erg03.** This neutron input file was generated with a fission KCODE card to allow neutron energies to range the spectrum. The unperturbed tallies should be identical, and both perturbed tallies should give identical answers (pert1 on tally4 and pert2 on tally14).

Godiva problem in LA-13374 on pg 30 used to check response to erg option  
c no expected response since reaction 16 has cutoff at 5.35 MeV

```

1 1 0.0479813 -1
2 0      1

1 so 8.741

kcode 1000 1.0 10 40
ksrc 0 0 0
imp:n 1 0
m1 92235.50c 1
f4:n 1
fm4 -1 1 16:17
sd4 1
f14:n 1
fm14 -1 1 16
sd14 1
pert1:n cell=1 rho=0.04 method=1 rxn=16 17 erg=5.5,9
pert2:n cell=1 rho=0.04 method=1 rxn=16   erg=5.5,9
prdmp 2j -1

```

## G. Effect on Tally Types 6 and 7

These input files test the effect of the new capability on tally types 6 and 7 by using neutron and photon problems. The correction is applied since these are cross-section dependent tallies. A pair of files is created, the first file has a type 6 or 7 tally, and the second uses an equivalent type 4 tally with an FM card. By including a negative multiplicative constant on the FM card, the correction will be applied to the type 4 tally file, and then this perturbed tally should match the type 6 or 7 tally from the first file.

**1. Input File Tal61.** This neutron KCODE problem includes a type 6 tally, and its tally result should match the corrected perturbed tally results from the following problem, tal61b.

Godiva problem in LA-13374 on pg 30 used to check response to type 6 tally

```

1 1 0.0479813 -1
2 0      1

1 so 8.741

kcode 1000 1.0 10 300
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
f6:n 1
sd6 1
prdmp 2j -1

```

**2. Input File Tal61b.** This neutron KCODE problem includes an equivalent type 4 tally with a tally multiplier card. Its tally result should match the corrected perturbed tally results from the previous problem, tal61.

Replace tal61 cell 1 definition (line 2) with:

```
1 1 0.0485 -1
```

Replace tal61 tally section (lines 11-12) with:

```
f4:n 1
fm4 -1 1 -1 -4
sd4 1
```

Add to tal61 the following perturbation definition:

```
pert1:n cell=1 rho=0.0479813 method=-1 rxn=-1
```

**3. Input File Tal62.** This neutron and photon KCODE problem includes a type 6 tally. Its tally result should match the corrected perturbed tally results from the following problem, tal62b.

Godiva problem in LA-13374 on pg 30 used to check response to type 6 tally

```
1 1 0.0479813 -1
```

```
2 0 1
```

```
1 so 8.741
```

```
mode n p
kcode 1000 1.0 10 300
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
f6:n 1
sd6 1
f16:p 1
sd16 1
prdmp 2j -1
```

**4. Input File Tal62b.** This neutron and photon KCODE problem includes an equivalent type 4 tally with a tally multiplier card. Its tally results for neutrons and photons should match the type 6 tally results from the previous problem, tal62.

Replace tal62 cell 1 definition (line 2) with:

```
1 1 0.048 -1
```

Replace the tally section (lines 12-15) in tal62 with:

```
f4:n 1
fm4 -1 1 -1 -4
sd4 1
f14:p 1
fm14 -1 1 -5 -6
```

```
sd14 1
```

Add the following two perturbation definitions to tal62.

```
pert1:n cell=1 rho=0.0479813 method=-1 rxn=-1
pert2:p cell=1 rho=0.0479813 method=-1 rxn=-5
prdmp 2j -1
```

**5. Input File Tal63.** This photon problem includes a type 6 tally, and its tally result should match the corrected perturbed tally results from the following problem, tal63b.

Godiva problem in LA-13374 on pg 30 used to check response to type 6 tally

```
1 1 0.0479813 -1
2 0 1

1 so 8.741

mode p
sdef erg=d1 pos=0 0 0
s1 0 14
sp1 0 1
nps 100000
imp:p 1 0
m1 92235 -94.73 92238 -5.27
f6:p 1
sd6 1
prdmp 2j -1
```

**6. Input File Tal63b.** This photon problem includes an equivalent type 4 tally with a tally multiplier card. Its tally result should match the type 6 tally results from the previous problem, tal63.

Replace tal63 cell 1 definition (line2) with:

```
1 1 0.047 -1
```

Replace tal63 tally section (lines 14-15) with:

```
f4:p 1
fm4 -1 1 -5 -6
sd4 1
f14:p 1
fm14 0.047 1 -5 -6
sd14 1
```

Add the following perturbation definition to tal63:

```
pert1:p cell=1 rho=0.0479813 method=-1 rxn=-5
```

**7. Input File Tal71.** This neutron KCODE problem includes a type 7 tally, and its tally result should match the corrected perturbed tally results from the following problem, tal71b.

Godiva problem in LA-13374 on pg 30 used to check response to type 7 tally

```
1 1 0.0479813 -1
```

```
2 0      1
```

```
1 so 8.741
```

```
kcode 1000 1.0 10 800
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
f7:n 1
sd7 1
prdmp 2j -1
```

**8. Input File Tal71b.** This neutron KCODE problem includes an equivalent type 4 tally with a tally multiplier card. Its tally result should match the type 7 tally results from the previous problem, tal71.

Replace tal71 cell 1 definition (line2) with:

```
1 1 0.0485 -1
```

Replace tal71 tally section (lines 14-15) with:

```
f4:n 1
fm4 -1 1 -6 -8
sd4 1
```

Add the following perturbation definition to tal71.

```
pert1:n cell=1 rho=0.0479813 method=-1 rxn=-6
```

## H. Perturbation Convergence

These files are combinations of earlier presented files and are used to test convergence of the perturbation to the expected value. The first file of the pair calculates a perturbation, whether it be density, material, or otherwise. The second file is a copy of the first file but replaces the relevant information from the first file's perturbation definition. Both files are then run to convergence and the tallies compared. If the perturbation is converging properly, it is expected that the tallies will be very close.

**1. Input File Fm71.** This neutron KCODE problem sets up a material perturbation. The perturbed tally results of PERT1 should match the tally results from fm71b. The results from PERT2 gives an idea of how much the first- and second-order perturbation terms contribute.

```
test for convergence
1 1 0.0479813 -1
2 0      1
```

```
1 so 8.741
```

```
kcode 5000 1.0 20 5000
```

```

ksrc 0 0 0
imp:n 1 0
m1 92235 -94.73 92238 -5.27
m2 92235 -87 92238 -13
f4:n 1
fm4 -1 1 -6 -7:-2
sd4 1
pert1:n cell=1 mat=2 method=-1 rxn= -6 -2
pert2:n cell=1 mat=2 method=3 rxn= -6 -2
prdmp 2j -1
dbcn

```

**2. Input File Fm71b.** This neutron KCODE problem generates the expected values for the perturbed tally from the previous problem.

Replace fm71 material section (lines 10-11 ) with:  
m1 92235 -87 92238 -13

Delete the PERT cards from fm71

**3. Input File Fm72.** This photon problem checks the density perturbation convergence of nonsequentially numbered cells and nonsequentially perturbed cells. The perturbed tally results of PERT1 should match the tally results from fm72b. The results from PERT2 gives an idea of how much the first- and second-order perturbation terms contribute. PERT3 is a check of cell 4 and a list of reactions.

```

test for convergence
1 1 0.0479813 -1
15 1 0.0479813 1 -215 -216 217
4 1 0.0479813 -23 (215: 216 : -217)
35 0 23

```

```

1 so 2
215 cx 3
216 px 5
217 px -4
23 so 8

```

```

sdef rad d1 pos 0 0 0
si1 0 2
sp1 -21 2
imp:p 1 1 1 0
mode p
nps 100000
m1 92235 -94.73 92238 -5.27
f4:p 1
f14:p 15
f24:p 4
fm4 -1 1 -4:-3
fm14 (-1 1 -5) (-1 1 -2:-3) (1 1 -6)

```

```
fm24 -1 1 -2:-3:-4
sd4 1
sd14 1
sd24 1
pert1:p cell=1 rho=0.0485 method=-1 rxn= -4 -3
pert2:p cell=1 rho=0.0485 method=-2 rxn= -4 -3
pert3:p cell=4 rho=0.0485 method=-1 rxn= -4 -2 -3
prdmp 2j -1
```

**4. Input File Fm72b.** This photon problem generates the expected values from the perturbation tests in the previous problem.

Substitute the first cell definitions (lines 2-4) in fm72 with:

```
1 1 0.0485 -1
15 1 0.0485 1 -215 -216 217
4 1 0.0485 -23 (215: 216 : -217)
```

Delete the PERT cards in fm72.

**5. Input File Fm73.** This neutron KCODE problem is a density perturbation. The first perturbation calculates the entire perturbation, whereas the second one calculates only the second-order perturbation.

Godiva problem in LA-13374 on pg 30 with Carter's suggested tests

```
1 1 0.0479813 -1
2 0 1

1 so 8.741

kcode 5000 1.0 10 5000
ksrc 0 0 0
imp:n 1 0
m1 92235.50c -94.73 92238.50c -5.27
f4:n 1
fm4 -1 1 -6 -7
sd4 1
pert1:n cell=1 rho=.053 method=1
pert2:n cell=1 rho=.053 method=3
prdmp 2j -1
```

**6. Input File Fm73b.** This problem generates the expected values for the perturbed tally in fm73.

Replace the cell 1 definition (line 2) in fm73 with:

```
1 1 0.053 -1
```

Delete the PERT cards in fm73.

**7. Input File Fm75.** This neutron problem uses a density perturbation as well as a material perturbation. The material that is being perturbed to is simply a repeated nuclide, so no difference between the two perturbed results is expected.

Godiva problem in LA-13374 on pg 30 used to compare converged repeated nuclide response

1 1 0.0479813 -1

2 0 1

1 so 8.741

```
kode 5000 1.0 10 5000
ksrc 0 0 0
imp:n 1 0
m1 92235.50c 0.5 92238.50c 0.5
m2 92235.50c 0.1 92235.50c 0.4 92238.50c 0.5
f4:n 1
fm4 -1 1 1
sd4 1
pert1:n cell=1 mat=1 rho=0.05 method=1
pert2:n cell=1 mat=1 rho=0.05 method=2
pert3:n cell=1 mat=2 rho=0.05 method=1
pert4:n cell=1 mat=2 rho=0.05 method=2
prdmp 2j -1
```

**8. Input File Fm75b.** This problem generates the expected values for the perturbed tally in fm75.

Replace the cell1 definition (line 2) in fm75 with:

1 1 0.05 -1

Delete the PERT cards in fm75.



## APPENDIX B

### CROSS-SECTION DEPENDENT TALLY VERIFICATION INPUT FILES

This appendix is taken from Ref. 3 and is listed here for completeness. The input files for the test problems discussed in Section VI are listed here. For each example, five input files are needed. The first file contains four perturbations and gives the unperturbed result. The remaining four files give the “actual” MCNP results for the perturbations by running with the perturbed densities and/or concentrations. The input files used to obtain “actual” results are listed here as alterations of the perturbed input file.

#### I. GODIVA-DENSITY PERTURBATION

The input for the unperturbed problem, `input=godiva1`, is

```
Godiva pert-back
1 1 -18.74 -1
2 0 1

1 so 8.741

kcode 3000 1.0 20 220
ksrc 0 0 0
imp:n 1 0
m1 92235 -94.73 92238 -5.27
f4:n 1
fn4 (-1 1 -6 -7)
sd4 1
pert1:n cell=1 rho=-20 method=2
pert2:n cell=1 rho=-20 method=1
pert3:n cell=1 rho=-21 method=2
pert4:n cell=1 rho=-21 method=1
pert5:n cell=1 rho=-23.5 method=2
pert6:n cell=1 rho=-23.5 method=1
pert7:n cell=1 rho=-26 method=2
pert8:n cell=1 rho=-26 method=1
```

The “actual” results for the four perturbations are obtained by deleting the PERT cards and changing the density of cell 1 on line 2,

```
1 1 -18.74 -1
```

with the first perturbation, `input=godiva2`,

```
1 1 -20 -1
```

or with the second perturbation, input=godiva3,

1 1 -21 -1

or with the third perturbation, input=godiva4,

1 1 -23.5 -1

or with the fourth perturbation, input=godiva5,

1 1 -26 -1

## II. GODIVA-COMPOSITION CHANGE

The input for the unperturbed problem, input=gconc1, is

Godiva concentration

1 1 -18.74 -1

2 0 1

1 so 8.741

```
rcode 3000 1.0 20 220
ksrc 0 0 0
imp:n 1 0
m1 92235 -94.73 92238 -5.27
m2 92235 -87 92238 -13
m3 92235 -74 92238 -26
m4 92235 -62 92238 -38
m5 92235 -50 92238 -50
m6 92235 -1
m7 92238 -1
f4:n 1
fm4 (-1 1 -6 -7)
  (-0.947931 6 -6 -7)
  (-0.052069 7 -6 -7)
sd4 1
pert1:n cell=1 rho=-18.74 mat=2 method=2
pert2:n cell=1 rho=-18.74 mat=2 method=1
pert3:n cell=1 rho=-18.74 mat=3 method=2
pert4:n cell=1 rho=-18.74 mat=3 method=1
pert5:n cell=1 rho=-18.74 mat=4 method=2
pert6:n cell=1 rho=-18.74 mat=4 method=1
pert7:n cell=1 rho=-18.74 mat=5 method=2
pert8:n cell=1 rho=-18.74 mat=5 method=1
```

The "actual" results for the four perturbations are obtained by deleting the PERT cards and replacing material 1 of cell 1 (line 2) and the FM card (lines 18 - 20),

```
1 1 -18.74 -1  
fm4 (-1 1 -6 -7) (-0.947931 6 -6 -7) (-0.052069 7 -6 -7)
```

with the first perturbation using material 2, input=gconc2,

```
1 2 -18.74 -1  
fm4 (-1 2 -6 -7)
```

or with the second perturbation using material 3, input=gconc3,

```
1 3 -18.74 -1  
fm4 (-1 3 -6 -7)
```

or with the third perturbation using material 4, input=gconc4,

```
1 4 -18.74 -1  
fm4 (-1 4 -6 -7)
```

or with the fourth perturbation using material 5, input=gconc5,

```
1 5 -18.74 -1  
fm4 (-1 5 -6 -7)
```

### III. TEST PROBLEM INP18-K<sub>eff</sub> ESTIMATE

The input for the unperturbed problem, input=inp181, is

```
testprob18 -- kcode in a hexagonal prism lattice.  
c three half control rods and five whole control rods.  
30 0 -905 -19 29 1 fill=1  
31 0 -906 -19 29 1 fill=1 (16.7113 0 0)  
37 0 -907 -19 29 1 fill=1 (-16.7113 0 0)  
34 0 -913 -19 29 fill=1 (0 11.9185 0)  
32 0 -914 -19 29 fill=1 (10.3217 5.9592 0)  
33 0 -915 -19 29 fill=1 (8.3557 14.4724 0)  
35 0 -916 -19 29 fill=1 (-8.3557 14.4724 0)  
36 0 -917 -19 29 fill=1 (-10.3217 5.9592 0)  
c universe 1: structure of control rod.  
38 11 -2.02 -880 u=1 $ control rod core  
39 6 -8.4 880 -881 u=1 $ control rod cladding  
40 12 -1.00 881 -882 u=1 $ control rod gap  
41 6 -8.4 882 u=1 $ control rod sheath  
c the space between the control rods, filled with lattice.  
140 0 -17 1 29 -19 905 906 907 913 914 915 916 917 fill=2
```

c universe 2: lattice of fuel rods with water in between.  
42 12 -1.00 -301 302 -303 304 -305 306 u=2 lat=2 fill=

-37:27 -1:33 0:0 &

2 4r 3 9r 2 4r 3 11r 2 4r 3 11r 2 4r 3 9r 2

2 4r 3 9r 2 3r 3 12r 2 3r 3 12r 2 3r 3 9r 2 1r

2 3r 3 10r 2 2r 3 13r 2 2r 3 13r 2 2r 3 10r 2 1r

2 3r 3 57r 2 2r &

2 2r 3 58r 2 2r

2 2r 3 16r 2 2r 3 17r 2 2r 3 16r 2 3r

2 2r 3 15r 2 3r 3 16r 2 3r 3 15r 2 4r

2 1r 3 15r 2 4r 3 15r 2 4r 3 15r 2 4r

2 1r 3 15r 2 3r 3 16r 2 3r 3 15r 2 5r

2 1r 3 15r 2 2r 3 17r 2 2r 3 15r 2 6r

2 1r 3 54r 2 7r &

c can code remember & thru comment?

2 3 55r 2 7r

2 3 25r 2 2r 3 25r 2 8r

2 3 24r 2 3r 3 24r 2 9r

2 3 23r 2 4r 3 23r 2 10r

2 3 15r 2 2r 3 4r 2 3r 3 4r 2 2r 3 15r 2 11r

2 3 14r 2 3r 3 4r 2 2r 3 4r 2 3r 3 14r 2 12r

2 3 13r 2 4r 3 11r 2 4r 3 13r 2 13r

2 3 13r 2 3r 3 12r 2 3r 3 13r 2 14r

2 3 13r 2 2r 3 13r 2 2r 3 13r 2 15r

2 3 46r 2 16r

2 3 45r 2 17r

2 3 44r 2 18r

2 1r 3 41r 2 20r

2 1r 3 40r 2 21r

2 1r 3 39r 2 22r

2 2r 3 36r 2 24r

2 2r 3 35r 2 25r

2 3r 3 32r 2 27r

2 4r 3 29r 2 29r

2 5r 3 26r 2 31r

2 6r 3 23r 2 33r

2 8r 3 18r 2 36r

2 11r 3 11r 2 40r

2 64r

c universe 3: structure of fuel rod lattice elements.

154 2 -13.75 -58 u=3 \$ fuel element

149 12 -1.00 58 -268 u=3 \$ gap

144 7 -19.66 268 -478 u=3 \$ liner

159 6 -8.4 478 -698 u=3 \$ cladding

141 12 -1.00 698 u=3 \$ water between the fuel rods

162 0 17:-29:19:-1 \$ outside world

\*1 py 0 \$ x-z plane, reflective

17 cz 29.135

19 pz 31.75 \$ top of reactor

29 pz -31.75 \$ bottom of reactor

58 c/z 3.4414 .8515 .3240

268 c/z 3.4414 .8515 .3345

478 c/z 3.4414 .8515 .3475

```

698 c/z 3.4414 .8515 .4318
880 cz 1.7251
881 cz 1.8051
882 cz 1.9051
905 cz 2.1055
906 c/z 16.7113 0 2.1055
907 c/z -16.7113 0 2.1055
913 c/z 0 11.9185 2.1055
914 c/z 10.3217 5.9592 2.1055
915 c/z 8.3557 14.4724 2.1055
916 c/z -8.3557 14.4724 2.1055
917 c/z -10.3217 5.9592 2.1055
301 px 3.9330
302 px 2.9498
303 p 1 1.7320508076 0 5.8994
304 p 1 1.7320508076 0 3.9330
305 p -1 1.7320508076 0 -.9834
306 p -1 1.7320508076 0 -2.9498

imp:n 1 18r 0
m2 92235.50d -.70573 92238.40c -.23821 7014.50d -.05605
m6 41093.40c -1.00000
m7 74000.55d -.74000
m11 5010.03d -.6870 5011.40c -.0840 6012.40c -.2290
m12 1001.60c 1 1002.60c 3 8016.40c 1
mt12 hwtr.01 lwtr.01
c pert1:n cell=42,141,40,149 rho=-1.50
kcode 2000 1 20 220
ksrc 3 2 2.2 3 2 -3 2 2.2 3 2 4 3 2 -4 3 2 4 3 1 -4 3 2
c e .01 .1 1. 10.
c fq f e
c fc4 fuel rod flux in 5 y locations averaged over 5 x elements
c f4:n (154<(42[-10:-6 -1 0])) $ average 5 x elements at j=-1
c (154<(42[-10:-6 3 0])) & $ average 5 x elements at j=3
c (154<(42[-10:-6 10 0])) $ average 5 x elements at j=10 &
c (154<(42[-10:-6 21 0])) $ average 5 x elements at j=21
c (154<(42[-10:-6 29 0])) $ average 5 x elements at j=29
c sd4 104.7089062 4r $ 5 times the volume of cell 154
c fm4 (1 2 -5) (1 2 -6) (1 2 -7) (1 2 -8) (1 2 4001) (1 2 102021)
print 30 90 102 110 160 161 162
c prdmp 2j -1
c ptrac buffer=20 file=asc write=all event=bnk
f14:n 154
fm14 (-1 2 -6 -7)
sd14 1
fc14 Keff estimator for cel 154
pert1:n cell=154 rho=-15.5 method=2
pert2:n cell=154 rho=-15.5 method=1
pert3:n cell=154 rho=-17 method=2
pert4:n cell=154 rho=-17 method=1
pert5:n cell=154 rho=-21.5 method=2
pert6:n cell=154 rho=-21.5 method=1
pert7:n cell=154 rho=-26 method=2
pert8:n cell=154 rho=-26 method=1

```

The "actual" results for the four perturbations are obtained by deleting the PERT cards and replacing the density of material 2, cell 154, line 58,

154 2 -13.75 -58 u=3 \$ fuel element

with the first perturbation, input=inp182,

154 2 -15.5 -58 u=3 \$ fuel element

or with the second perturbation, input=inp183,

154 2 -17. -58 u=3 \$ fuel element

or with the third perturbation, input=inp184,

154 2 -21.5 -58 u=3 \$ fuel element

or with the fourth perturbation, input=inp185,

154 2 -26. -58 u=3 \$ fuel element

#### IV. TEST PROBLEM INP02-NEUTRON ABSORPTION RATE ESTIMATE

The input for the unperturbed problem, input=inp021, is

testprob02 -- three different tallies of the same physical quantity.

1 1 -2.45 -1 \$pd5=.3 \$ boron ball with volume source  
2 2 -2.7 1 -2 4 \$pd5=1 \$ aluminum shell  
3 2 -2.7 2 -3 4 \$pd5=1 \$ aluminum shell  
4 0 3 \$pd5=1 \$ outside world  
5 2 -2.7 5 -4 \$pd5=1 \$ al. ball to av. dxtran/tally2 con.  
6 2 -2.7 -5 \$pd5=1 \$ little aluminum ball for tally 4

1 so 5  
2 so 7  
3 so 10  
4 sy 7 1.95  
5 sy 7 .3

c volume source in boron ball, biased in position.  
c the symmetry is sufficient for the bias to be a fair game.

sdef cel d4 x d1 y d2 z d3 erg=1  
si1 -5 5  
sp1 0 1  
sc2 position is biased toward the dxtran and the ring detector.  
si2 a -5 5  
sp2 1 1  
sb2 1 2

```

si3 -5 5
sp3 0 1
si4 1 1
sp4 v
c
m1 5010.00 .196 5011.40c .804 nlib=03d $ natural boron
m2 13027.40c 1 $ aluminum-27
m3 5010.0 .250 5011.40c .750 nlib .03d $ enriched b-10 of .250
c pert1:n cell=1 mat=3
c ctme 60
c phys:n 1.2 $ cross sections above 1.2 mev will be expunged.
c
c all tallies have the same energy bins.
c e0 .01 .03 .1 .3 1
c fc2 average flux on surface 2.
c f2:n 2
c f1:n 1
c c1 -.8 3i 0 4i 1 t
c fq1 c e
c tf1 1 7r
c ft2 tmc -2 .05
c t2 -2 9i 3 10 100
c fq2 t e
c ft1 frv 3 4 5 geb 1 2 0
fc4 neutron absorption in cell 6
f4:n 6
fm4 (-1 2 -2)
c dd5 .003
c fq5 u e
c fu5 1 8i 10
c ft5 inc
c fc5 average flux at ring detector.
c fy5:n 5 4.89 .7
c dxc:n 1 .7 .9 0 1 1
c dd1 .04 100
thtme -10 0 .5 1 2
# tmp1 tmp2 tmp3 tmp4 tmp5
1 1e-8 2e-8 3e-8 4e-8 5e-8
2 2e-8 3e-8 5e-8 4e-8 3e-8
3 1e-8 5e-8 4e-8 3e-8 2e-8
4 0 0 0 0 0
5 2e-8 1e-8 5e-8 3e-8 1e-8
6 3e-8 2e-8 1e-8 2e-8 1e-8
c
c dxt:n 0 7 0 1 1.9 $ dxtran around cell 6, inside cell 5.
imp:n 1 1 1 0 1 1
c
nps 10000000 $ run 5000 histories.
print 10 72 170
c prdmp 2500 625 -1 2 $ print mctal file.
c dbcn 14j 1
c ptrac buffer=2 file=asc event=src nps=1,200 cell=3
pert1:n cell=6 rho=-2.85 method=2
pert2:n cell=6 rho=-2.85 method=1

```

```
pert3:n cell=6 rho=-3 method=2
pert4:n cell=6 rho=-3 method=1
pert5:n cell=6 rho=-3.3 method=2
pert6:n cell=6 rho=-3.3 method=1
pert7:n cell=6 rho=-3.6 method=2
pert8:n cell=6 rho=-3.6 method=1
```

The "actual" results for the four perturbations are obtained by deleting the PERT cards and changing the density of cell 6, material 2, line 7,

```
6 2 -2.7 -5 $pd5=1 $ little aluminum ball for tally 4
```

with the first perturbation, input=inp022,

```
6 2 -2.85 -5 $pd5=1 $ little aluminum ball for tally 4
```

or with the second perturbation, input=inp023,

```
6 2 -3. -5 $pd5=1 $ little aluminum ball for tally 4
```

or with the third perturbation, input=inp024,

```
6 2 -3.3 -5 $pd5=1 $ little aluminum ball for tally 4
```

or with the fourth perturbation, input=inp025,

```
6 2 -3.6 -5 $pd5=1 $ little aluminum ball for tally 4
```

## V. TEST PROBLEM INP04-PHOTON COLLISION RATE ESTIMATE

The input for the unperturbed problem, input=inp041, is

```
testprob04 -- photons
1 1 .02 -1 $ uranium hydride ball with point source
2 2 .1 -2 1 3 4 $ uranium-lithium shell
3 0 2 $ zero-importance outside world
4 2.1 -3 5
5 2.1 -4 6
6 2.1 -5
7 2.1 -6

1 so 10
2 so 20
3 s -10 2r 2.1
4 s 10 2r 1.1
5 s -10 2r 1.9
6 s 10 2r .9
```

```

mode p
imp:p 1 1 0 1 1 1m 1m
m1 plib=02p 92000 1 1000 3
m2 92000 1 3000 3
m3 92000 0.9 3000 3.1
m4 92000 0.7 3000 3.3
m5 92000 0.5 3000 3.5
m6 92000 0.3 3000 3.7
m7 92000 1
m8 3000 1
c monoenergetic isotropic point source at (0,0,0)
sdef erg=d1 cel=1
sp1 -4
c e0 .01 .1 1 5
c f6:p 1 2 6 7 $ heating tally
c f5x:p 12 15 1
fc4 collisions in ULi Shell
c f4:p 1 2 6 7 $ flux tally
f4:p 2
fm4 (-1 2 -5)
(-0.25 7 -5)
(-0.75 8 -5)
c fq4 e f
c ft4 tmc -2 .05
c ft5 tmc -2 .05
c t4 -2 9i 3 10 100
c t5 -2 9i 3 10 100
c fq6 f e
c fq5 e d
c fq25 e d
c fz25:p -12 15 -1 -7 7 2
c dd 0 100 .01
c dd5 -.1
nps 1000000
c print 30 160 161 162
c prdmp 2j -1
c de4 1 10 100
c df4 0.8 0.9 1.0
c dxt:p -10 2r 1 2 10 2r 1 1 .01 .005
c dxc:p 1 1 0 .9 .9 .1 .1
c pd 1 1 0 .1 3r
c dd2 0 100 .005 .4m
c de25 .01 8i .1 8i 1 2
c df25 lin .8 18i .99
c dd1 -0.01 1000
c phys:p .05
c cf4 4
c cf6 5
c cut:p .1 .01 .5 .2 .8
pert1:p cell=2 rho=0.1 mat=3 method=2
pert2:p cell=2 rho=0.1 mat=3 method=1
pert3:p cell=2 rho=0.1 mat=4 method=2
pert4:p cell=2 rho=0.1 mat=4 method=1
pert5:p cell=2 rho=0.1 mat=5 method=2

```

```
pert6:p cell=2 rho=0.1 mat=5 method=1
pert7:p cell=2 rho=0.1 mat=6 method=2
pert8:p cell=2 rho=0.1 mat=6 method=1
print
```

The "actual" results for the four perturbations are obtained by deleting the PERT cards and replacing material 2 of cell 2 (line 3) and the FM card (lines 36 - 38),

2 2 .1 -2 1 3 4 \$ uranium-lithium shell

fm4 (-1 2 -5)  
(-0.25 7 -5)  
(-0.75 8 -5)

with the first perturbation using material 3, input=inp042,

2 3 .1 -2 1 3 4 \$ uranium-lithium shell

fm4 (-1 3 -5)

or with the second perturbation using material 4, input=inp043,

2 4 .1 -2 1 3 4 \$ uranium-lithium shell

fm4 (-1 4 -5)

or with the third perturbation using material 5, input=inp044,

2 5 .1 -2 1 3 4 \$ uranium-lithium shell

fm4 (-1 5 -5)

or with the fourth perturbation using material 6, input=inp045,

2 6 .1 -2 1 3 4 \$ uranium-lithium shell

fm4 (-1 6 -5)

## VI. TEST PROBLEM INP10-PHOTON COLLISION RATE ESTIMATE

The input for the unperturbed problem, input=inp101, is

```
testprob10 general test problem /x6code/gtprob
1 1 -6.4 1 -2 -31 32 -33 34
2 0 10 -4 -12 #1
3 2 -1 4 -14 -12 5
4 3 -8.94 -5 6
5 0 -6
```

```

6 4 -2.25 7 -8 -12
7 2 -1 8 -9 -12
8 2 -1 9 -12
9 4 -2.25 11 -10 -12
10 2 -1 -11 -12
11 3 -8.94 12 -13
12 0 13
13 2 -1 14 -7 -12 5

```

```

1 px 0
2 px 10
4 px 11.9
5 tx 30 0 0 20 18 18
6 tx 30 0 0 20 15 15
7 px 50
8 px 70
9 px 90
10 px -20
11 px -50
12 cx 40
13 cx 45
14 px 30
20 cx 10
21 cx 25
31 py 5
32 py -5
33 pz 5
34 pz -5

```

```

mode n p
m1 29000.02 1 8016.40 1
m2 1001.60 2 8016.40 1
m3 29000.02 1
m4 6012.40 1
imp:n 1 1 2 2 2 4 2 1 .25 1 0 4
imp:p 1 1 2 2 2 4 2 1 .25 1 0 4
sdef erg=d1 vec=1 0 0 dir=d2 pos=5 0 0 rad=d3 cel=1
sp1 -3
sb2 -31 1.2
si3 8.67
c f4:n 6
f14:p 6
fm14 (-1 4 -5)
fq s e
c fs -20 -21
phys:n j 1e-6
phys:p 1 0
nps 2000000
c prdmp 2j -1
print 50
pert1:n,p cell=6 rho=-2.4 method=2
pert2:n,p cell=6 rho=-2.4 method=1
pert3:n,p cell=6 rho=-2.6 method=2
pert4:n,p cell=6 rho=-2.6 method=1

```

```
pert5:n,p cell=6 rho=-3.0 method=2
pert6:n,p cell=6 rho=-3.0 method=1
pert7:n,p cell=6 rho=-3.6 method=2
pert8:n,p cell=6 rho=-3.6 method=1
```

The "actual" results for the four perturbations are obtained by deleting the PERT cards and changing the density of cell 6, material 4, line 7,

6 4 -2.25 7 -8 -12

with the first perturbation, input=inp102,

6 4 -2.4 7 -8 -12

or with the second perturbation, input=inp103,

6 4 -2.6 7 -8 -12

or with the third perturbation, input=inp104,

6 4 -3.0 7 -8 -12

or with the fourth perturbation, input=inp105,

6 4 -3.6 7 -8 -12

## APPENDIX C

### EXAMPLE PERTURBATION PROBLEMS

#### I. OVERVIEW

This appendix is taken from Ref. 2 and is shown here for completeness. The perturbation problems previously presented in this report are mainly focused upon verification of the new tally-dependent cross-section capability. The examples given in this appendix represent perturbations designed to demonstrate the PERT card capability of voiding and unvoiding regions as well as composition changes.

#### A. Voiding and Unvoiding

Voiding a cell is simply an extension of a density change, using the keywords CELL and RHO on the PERT card, with the density set to zero. Unvoiding a cell cannot be directly performed using this technique; however, a simple solution is to include the material in the unperturbed problem. In this approach, the cell of interest is modeled with the material, and the PERT card simply voids the cell. The sign of the perturbation results should be reversed in the case of unvoiding. The following MCNP example includes a sphere of  $\text{UH}_3$  surrounded by a void spherical shell and a layer of  $\text{ULi}_3$ .

```
Appendix C sample problem 1
1 1 .02 -1 imp:p=1 $ UH3 inner sphere
2 0 1 -2 imp:p=1 $ Void spherical shell
3 2 .1 2 -3 imp:p=1 $ ULi3 outer shell
4 0 3 imp:p=0 $ Outside world

1 so 10
2 so 10.5
3 so 20

mode p
m1 92000 1 1000 3    $ Uranium Hydride
m2 92000 1 3000 3    $ Uranium Lithium
sdef erg=6            $ 6 MeV source at center
f1:p 3                $ Current on outer surface
nps 25000
```

To unvoid cell 2 with  $ULi_3$ , simply fill cell 2 with  $ULi_3$ , add a PERT card that voids cell 2, and reverse the sign of the perturbation estimate for Tally 1. These modifications are included in the following input file and denoted by the arrows.

```
Appendix C sample problem 1
1 1 .02 -1 imp:p=1 $ UH3 inner sphere
→ 2 2 .1 1 -2 imp:p=1 $ ULi3 inner shell
3 2 .1 2 -3 imp:p=1 $ ULi3 outer shell
-- 4 0 3 imp:p=0 $ Outside world

1 so 10
2 so 10.5
3 so 20

mode p
m1 92000 1 1000 3      $ Uranium Hydride
m2 92000 1 3000 3      $ Uranium Lithium
→ pertl:p cell=2 rho=0.
sdef erg=6              $ 6 MeV source at center
f1:p 3                  $ Current on outer surface
nps 25000
```

Clearly if one wants to unvoid a region with several different materials, then separate runs must be performed.

## B. Composition and Geometric Perturbations

A composition perturbation can range from a slight variation in atom or weight fractions to a change in material. Variations in atom or weight fractions are straightforward and require only an additional material card, reflecting the fractional changes, and the use of the CELL and MAT keywords on the PERT card (the RHO keyword may also be used to alter the density). Changes in material, on the other hand, are somewhat more complicated. In this case, the unperturbed problem must be modified such that cells of interest contain a mixture of both materials (the original material plus the perturbation material). Furthermore, two PERT cards are required to estimate the change back to the original material *and* to the perturbation material. Finally, these two perturbation results must be properly combined to obtain the overall estimate for the material perturbation.

Consider the previous example, except that this time cell 2 is filled with  $UH_3$ .

```
Appendix C sample problem 2
1 1 .02 -1 imp:p=1 $ UH3 inner sphere
```

```

2 1 .02 1 -2 imp:p=1 $ UH3 inner shell
3 2 .1 2 -3 imp:p=1 $ ULi3 outer shell
4 0 3 imp:p=0 $ Outside world

1 so 10
2 so 10.5
3 so 20

mode p
m1 92000 1 1000 3 $ Uranium Hydride
m2 92000 1 3000 3 $ Uranium Lithium
sdef erg=6 $ 6 MeV source at center
f1:p 3 $ Current on outer surface
nps 25000

```

The effect of changing cell 2 from UH<sub>3</sub> to ULi<sub>3</sub> can be estimated with the following steps. First, fill cell 2 with a mixture of UH<sub>3</sub> and ULi<sub>3</sub>. The new material card needed for this cell can be obtained by simply adding the atom fractions of the separate materials. This same approach can be used for weight fractions as well. As long as a significant amount of each material is in the mixture, the way they are combined is not important. Next, add two PERT cards — one that perturbs cell 2 back to UH<sub>3</sub> and one that perturbs cell 2 to ULi<sub>3</sub>. This leads to the following input file with the changes denoted by the arrows.

```

Appendix C sample problem 2
1 1 .02 -1 imp:p=1 $ UH3 inner sphere
→ 2 3 .06 1 -2 imp:p=1 $ Mixture of UH3 and ULi3
3 2 .1 2 -3 imp:p=1 $ ULi3 outer shell
4 0 3 imp:p=0 $ Outside world

1 so 10
2 so 10.5
3 so 20

mode p
m1 92000 1 1000 3 $ Uranium Hydride
m2 92000 1 3000 3 $ Uranium Lithium
→ m3 92000 2 1000 3 3000 3 $ Half UH3 and ULi3
→ pert1:p cell=2 mat=1 rho=.02
→ pert2:p cell=2 mat=2 rho=.1
sdef erg=6 $ 6 MeV source at center
f1:p 3 $ Current on outer surface
nps 25000

```

Note that the density of cell 2 is consistent with the mixture of UH<sub>3</sub> and ULi<sub>3</sub>. The exact value of this density is not important, as long as it is between the densities of the two materials. It

should also be noted that the unperturbed results for Tally 1 will change from that of the previous input file, since they are now consistent with the mixture of materials in cell 2. Finally, properly combining the perturbation results is important. To estimate the change of going *from*  $\text{UH}_3$  *to*  $\text{ULi}_3$ , take PERT2 minus PERT1. To estimate the change of going *from*  $\text{ULi}_3$  *to*  $\text{UH}_3$ , take PERT1 minus PERT2.

Geometric perturbations are included in this section since they can be modeled, in most cases, as material perturbations. Such perturbations are achieved in MCNP by overspecifying the geometry in the region of interest. For example, the previous problem can be viewed as a geometric perturbation in that it gives the estimated effect of the  $\text{ULi}_3$  region collapsing into the  $\text{UH}_3$  region. In a similar manner, one could consider the effect of withdrawing a control rod in a nuclear reactor. Simply model the region of motion as a separate cell and perturb the material in that cell from control rod material to moderator material, for example.

## APPENDIX D

### PERTURBATION ERRORS IN MCNP4B

#### I. ERRORS ENCOUNTERED

During the testing of the new perturbation correction capability, it was determined that three errors existed in the perturbation feature of MCNP4B. The first error identified by these tests concerns repeated nuclides. It was possible to create a simple problem for which no perturbation would be expected but one resulted. A test set (see next section) was generated by using a repeated nuclide with fractions that sum to the same total as given on a previous material card:

```
M1 92235 0.5 92238 0.5  
M2 92235 0.4 92235 0.1 92238 0.5 .
```

Both M1 and M2, when used as the material for a cell, yield identical f4 tally results. However, if the tally was perturbed from M1 to M2 with a 0.04% density change, MCNP4B gave a large perturbation, sometimes on the order of 10000% of the unperturbed tally. This has been corrected in version 4C.

The second error involved the RXN parameter on the PERT card. The users' manual states that nonstandard special R numbers can be used to specify the reaction to be perturbed.<sup>1</sup> (These nonstandard special reaction numbers are listed in Section III.B.2.) However, when the special R number -1 was used in a neutron problem or if RXN=-5 was used for a photon problem, MCNP4B gave erroneous results. These cases had not been considered in the original programming of 4B. This, too, has been corrected in version 4C.

The RXN=-1 case for neutrons has been tested, and it gave the same corrected results as RXN=1 and no RXN specified (the default is assumed RXN=1).<sup>1</sup> The test problem which illustrates this is "mtfm01" (found in Appendix A Section II.A.1) which does show a difference in the perturbed tally in the last decimal place. The difference occurs since MT=1 includes thermal effects and MT=-1 does not. The RXN=-5 case for photons has also been corrected. The file "mtfm35" (found in Appendix A Section II.A.9) illustrates this change.

The third error was the missing  $2y_1y_2$  term in the  $\alpha_{j'k}$  of Eq. (36). The effect is small - usually unnoticeable. This has been corrected in version 4C.

## II. REPEATED NUCLIDE TEST SET

The following sections describe the repeated nuclide test set which was used and results obtained when the input files were run using MCNP versions 4B and 4C. To compare output results, it was necessary to turn the perturbation correction capability off. Thus, on the FM card for each of these problems, notice that a positive multiplicative constant is used.

### A. Input File Rep01

This neutron input file has a volume averaged tally on the default reaction (MT neutron reaction 1 on FM card) and only uses material 1 for cross-section data.

Godiva problem in LA-13374 on pg 30 used to check for repeated nuclides

```
1 1 0.0479813 -1  
2 0 1
```

```
1 so 8.741
```

```
kcode 1000 1.0 10 40  
ksrc 0 0 0  
imp:n 1 0  
m1 92235.50c 0.5 92238.50c 0.5  
m2 92235.50c 0.1 92235.50c 0.4 92238.50c 0.5  
f4:n 1  
fm4 0.0479813 1 1  
sd4 1  
prdmp 2j -1
```

The results (with error given in relative error) obtained for this tally are:

4B: 3.17534E+00 ± 0.0014

4C: 3.17534E+00 ± 0.0014

These results match as are expected and will be referred to as nominal case 1.

### B. Input File Rep02

This neutron input file has a volume averaged tally on the default reaction (MT neutron reaction 1 on FM card) and only uses material 2 for cross-section data.

Replace the material 1 card (line 2) in rep01 with:

```
1 2 0.0479813 -1
```

Replace the FM card (line 13) in rep01 with:

```
fm4 0.0479813 2 1
```

The results (with error given in relative error) obtained for this tally are:

4B: 3.17534E+00  $\pm$  0.0014

4C: 3.17534E+00  $\pm$  0.0014

These results match as expected; furthermore, they match the results of nominal case 1. The results of rep02 will be referred to as nominal case 2.

### C. Input File Rep03

This neutron input file has a volume averaged tally on the default reaction (MT neutron reaction 1 on FM card) and only uses material 1 for cross-section data. This problem will calculate the tally which should be expected if the slight density change is used.

Replace the material 1 card (line 2) in rep01 with:

1 2 0.048 -1

Replace the FM card (line 13) in rep01 with:

fm4 0.048 2 1

The results (with error given in relative error) obtained for this tally are:

4B: 3.17701E+00  $\pm$  0.0014

4C: 3.17701E+00  $\pm$  0.0014

These results match as expected; furthermore, they seem consistent with the logic that a very small increase in density (0.04%) of the material will result in a very small increase in the tally on all reaction types. The results of rep03 will be referred to as nominal case 3.

### D. Input File Rep04

This neutron input file has a volume averaged tally on the default reaction (MT neutron reaction 1 on FM card) and only uses material 1 for cross-section data. However, this problem adds a single perturbation from material 1 to material 2 with a slight density perturbation. (If no density perturbation is used, version 4C turns off the perturbation because it recognizes that material 1 is equivalent to material 2.) It is expected that the perturbation should be a very small value since the density was changed by about 0.04%.

Add the perturbation 1 card to rep01:

pert1:n cell=1 mat=2 rho=0.048

The results (with error given in relative error) obtained for the F4 tally are:

4B: 3.17534E+00  $\pm$  0.0014

4C: 3.17534E+00  $\pm$  0.0014

The results (with error given in relative error) obtained for perturbation 1 are:

4B: 2.58469E-01  $\pm$  0.0434

4C: 3.76813E-05  $\pm$  0.1363

The unperturbed tally results match those of nominal case 1 and 2, as was expected, since that part of the problem was unaffected by the perturbation. However, the perturbation results do not match. Version 4B calculates a large perturbation, whereas version 4C predicts a much smaller one. From nominal case 3, it is seen that this perturbation should be much smaller than that calculated by version 4B and on the order of the perturbation calculated by 4C.

## E. Input File Rep09

This photon input file has a volume averaged tally on the default reaction (FM photon reaction -5 on FM card) and only uses material 1 for cross-section data. This problem adds a single perturbation from material 1 to material 2 and a slight density perturbation. (If no density perturbation is used, version 4C turns off the perturbation because it recognizes that material 1 is equivalent to material 2.) It is expected that the perturbation should be a very small value, since the density was changed by about 0.04%.

Photon problem used to check repeated nuclides

1 1 0.0479813 -1  
2 0 1

1 so 8.741

```
mode p
nps 10000
sdef pos 0 0 0
imp:p 1 0
m1 92238 0.9 92235 0.09 1001 0.01
m2 92000 0.9 92000 0.09 1001 0.01
f4:p 1
fm4 0.0479813 1 -5
sd4 1
pert1:p cell=1 mat=2 rho=0.048
prdmp 2j -1
```

The results (with error given in relative error) obtained for the F4 tally are:

4B: 4.58160E+01  $\pm$  0.0030

4C: 4.58160E+01  $\pm$  0.0030

The results (with error given in relative error) obtained for perturbation 1 are:

4B: 5.67577E+03  $\pm$  0.0076

4C: 1.24394E-02  $\pm$  0.0170

These perturbed results do not match and are quite different! The version 4B perturbed tally is 2 orders of magnitude higher than the unperturbed tally. This is clearly incorrect since there was such a tiny density perturbation involved. However, version 4C (which has been corrected) yields values which are much more reasonable.



## APPENDIX E

### REVISED TEST SUITE INPUT FILES

The test suite problems are used to ensure that MCNP has been installed and compiled correctly. Changes between MCNP versions B and C necessitated changes in the test suite files to ensure that new capabilities are correctly installed. The following sections show the three changed test suite problems. Changed lines are denoted by an arrow.

#### I. NEW TEST SUITE PROBLEM INP10

```
testprob10 general test problem /x6code/gtprob
1 1 -6.4 1 -2 -31 32 -33 34
2 0 10 -4 -12 #1
3 2 -1 4 -14 -12 5
4 3 -8.94 -5 6
5 0 -6
6 4 -2.25 7 -8 -12
7 2 -1 8 -9 -12
8 2 -1 9 -12
9 4 -2.25 11 -10 -12
10 2 -1 -11 -12
11 3 -8.94 12 -13
12 0 13
13 2 -1 14 -7 -12 5

1 px 0
2 px 10
4 px 11.9
5 tx 30 0 0 20 18 18
6 tx 30 0 0 20 15 15
7 px 50
8 px 70
9 px 90
10 px -20
11 px -50
12 cx 40
13 cx 45
14 px 30
20 cx 10
21 cx 25
31 py 5
32 py -5
33 pz 5
34 pz -5

mode n p
m1 29000.02 1 8016.40 1
```

```

m2 1001.60 2 8016.40 1
m3 29000.02 1
m4 6012.40 1
→ m5 6012.40 0.4 6012.40 0.6
imp:n 1 1 2 2 2 4 2 1 .5 .25 1 0 4
imp:p 1 1 2 2 2 4 2 1 .5 .25 1 0 4
sdef erg=d1 vec=1 0 0 dir=d2 pos=5 0 0 rad=d3 cel=1
sp1 -3
sb2 -31 1.2
si3 8.67
f4:n 6
→ sd4 1 1 1
→ fm4 (-1 5 -1)
→ f14:p 6
→ sd14 1 1 1
→ fm14 (-1 5 -5)
→ pert1:p cell=6 rho=-2.2 method=-1 rxn=501
→ pert2:p cell=6 rho=-2.2 method=2 rxn=-5
→ pert3:p cell=6 rho=-2.2 mat=5 method=-1 rxn=-5
→ pert4:n cell=6 rho=-2.2 method=-1 rxn=-1
→ pert5:n cell=6 rho=-2.2 mat=5 method=-1 rxn=-1
fq s e
fs -20 -21
phys:n j 1e-6
phys:p 1 0
nps 500
prdmp 2j -1
print 50

```

## II. NEW TEST SUITE PROBLEM INP11

```

testprob11 -- intertwined super pretzels with s(a,b), mode n p
1 1 -7.8 -1:-2:-3 $ pretzel of tori
2 2 -2.66 -4:-5:-6:-7:-8:-9:-10:-11 $ cage of ellipsoids
3 3 -9 -12 -13:-14:-15:-16:-17:-18:-19:-20:-21 $ toys
4 4 -5 1 2 3 4 5 6 7 8 9 10 11(12:13) $ space between
14 15 16 17 18 19 20 21 -22
5 0 22 $ zero-importance outside world
6 0 -23 -24 -25 26 $ cookie-cutter cell

1 tx 0 0 0 1 0 2 2
2 ty 0 0 0 1 2 2 2.5
3 tz 0 0 0 1 0 3 4
4 sq .028 1 1 0 0 0 -1 0 1 5 5
5 sq 1 .00448 1 0 0 0 -1 -5 0 5
6 sq 1 1 .028 0 0 0 -1 -5 -15 0
7 sq 1 .00448 1 0 0 0 -1 -5 0 -5
8 sq .028 1 1 0 0 0 -1 0 1 5 -5
9 sq 1 .00448 1 0 0 0 -1 5 0 -5
10 sq 1 1 .028 0 0 0 -1 5 -15 0
11 sq 1 .00448 1 0 0 0 -1 5 0 5
12 sq .1 0 .05 0 1 0 -4 0 -11 17
13 sq .1 0 .07 0 -.3 0 -10 0 -1 16

```

```

14  sq .05 .2 1 0 0 0 -16 0 -6 -20
15  sq 1 .1 1 0 0 0 -4 0 14 -14
16  sq 1 1 .1 0 0 0 -4 0 14 -14
17  s 0 4.5 22.5 2
18  s 0 6.5 22.5 2
19  s 0 5.5 18 4
20  s 0 4.5 14 1
21  s 0 6.5 14 1
22  so 28
23  pz 9
24  c/y 1 .5 10
25  py -18.5
26  py -21.5

m1  92235.50d 1
m2  13027.40c 1  8016.40c 2
m3  29000.02c 1 4009.60c 1
m4  gas=1 1001.60c 2 8016.40c 1
m5  13027.26y 1
mt3  be.01t
mt4  h/zr.02t
pert1:n,p cell=1 rho=-8.75 $ 5% increase in tally 4
→ pert2:n,p cell=2 rho=-2.74 rxn=-1 $should give fatal error due to rxn
→ pert3:n cell=2 rho=-2.74 rxn=-1 -2 -3 -4 1 2
imp:n 1 1 1 1 0 0
mode n p
c  monodirectional source on plane with cookie cutter
sdef pos 0 -20 0 dir 1 vec .05 1 .1 rad d1 axs .05 1 .1 ara=0.0001
ccc 6 erg d2
s1  0 12
s2  1e-8 .001
sp2  0 1
cut:n 1000 0 .2 .1
fq  f e
f4:n 1 2 3
sd4  (1) (1) (1)
fc4  volumes=1. so tally is volume-integrated flux
e4  1e-7 .001 20
fm4 .98 5 103
f14:n 2
sd14 (1)
fm14 (1 2 -1) (1 2 -2) (1 2 -3) (1 2 -4) (1 2 1) (1 4 2)
→ f34:n 2
→ sd34 (1)
→ fm34 (-1 2 -1) (-1 2 -2) (-1 2 -3) (-1 2 -4) (-1 2 1) (-1 4 2)
f24:n 2
sd24 (1)
fm24 ((1.0023e-04 2 (102)(51)(52))(1.0 -1 2 0.000502))
f11:p 1 2 3 t
tmp1 4e-8 3r 0 0
f5:n 0 0 0 0
dxt:n 0 0 0 0.001 0.002
f15:p 0 0 0 0
nps 2500

```

```
PWt 1 1 -1 -1 -1 -1  
print 30 40  
prdmp 2j -1
```

### III. NEW TEST SUITE PROBLEM INP18

```
testprob18 -- kcode in a hexagonal prism lattice.  
c three half control rods and five whole control rods.  
30 0 -905 -19 29 1 fill=1  
31 0 -906 -19 29 1 fill=1 (16.7113 0 0)  
37 0 -907 -19 29 1 fill=1 (-16.7113 0 0)  
34 0 -913 -19 29 fill=1 (0 11.9185 0)  
32 0 -914 -19 29 fill=1 (10.3217 5.9592 0)  
33 0 -915 -19 29 fill=1 (8.3557 14.4724 0)  
35 0 -916 -19 29 fill=1 (-8.3557 14.4724 0)  
36 0 -917 -19 29 fill=1 (-10.3217 5.9592 0)  
c universe 1: structure of control rod.  
38 11 -2.02 -880 u=1 $ control rod core  
39 6 -8.4 880 -881 u=1 $ control rod cladding  
40 12 -1.00 881 -882 u=1 $ control rod gap  
41 6 -8.4 882 u=1 $ control rod sheath  
c the space between the control rods, filled with lattice.  
140 0 -17 1 29 -19 905 906 907 913 914 915 916 917 fill=2  
c universe 2: lattice of fuel rods with water in between.  
42 12 -1.00 -301 302 -303 304 -305 306 u=2 lat=2 fill=  
-37:27 -1:33 0:0 &  
2 4r 3 9r 2 4r 3 11r 2 4r 3 11r 2 4r 3 9r 2  
2 4r 3 9r 2 3r 3 12r 2 3r 3 12r 2 3r 3 9r 2 1r  
2 3r 3 10r 2 2r 3 13r 2 2r 3 13r 2 2r 3 10r 2 1r  
2 3r 3 57r 2 2r &  
2 2r 3 58r 2 2r  
2 2r 3 16r 2 2r 3 17r 2 2r 3 16r 2 3r  
2 2r 3 15r 2 3r 3 16r 2 3r 3 15r 2 4r  
2 1r 3 15r 2 4r 3 15r 2 4r 3 15r 2 4r  
2 1r 3 15r 2 3r 3 16r 2 3r 3 15r 2 5r  
2 1r 3 15r 2 2r 3 17r 2 2r 3 15r 2 6r  
2 1r 3 54r 2 7r &  
c can code remember & thru comment?  
2 3 55r 2 7r  
2 3 25r 2 2r 3 25r 2 8r  
2 3 24r 2 3r 3 24r 2 9r  
2 3 23r 2 4r 3 23r 2 10r  
2 3 15r 2 2r 3 4r 2 3r 3 4r 2 2r 3 15r 2 11r  
2 3 14r 2 3r 3 4r 2 2r 3 4r 2 3r 3 14r 2 12r  
2 3 13r 2 4r 3 11r 2 4r 3 13r 2 13r  
2 3 13r 2 3r 3 12r 2 3r 3 13r 2 14r  
2 3 13r 2 2r 3 13r 2 2r 3 13r 2 15r  
2 3 46r 2 16r  
2 3 45r 2 17r  
2 3 44r 2 18r  
2 1r 3 41r 2 20r  
2 1r 3 40r 2 21r  
2 1r 3 39r 2 22r
```

```

2 2r 3 36r 2 24r
2 2r 3 35r 2 25r
2 3r 3 32r 2 27r
2 4r 3 29r 2 29r
2 5r 3 26r 2 31r
2 6r 3 23r 2 33r
2 8r 3 18r 2 36r
2 11r 3 11r 2 40r
2 64r
c  universe 3: structure of fuel rod lattice elements.
154 2 -13.75 -58 u=3 $ fuel element
149 12 -1.00 58 -268 u=3 $ gap
144 7 -19.66 268 -478 u=3 $ liner
159 6 -8.4 478 -698 u=3 $ cladding
141 12 -1.00 698 u=3 $ water between the fuel rods
162 0 17:-29:19:-1 $ outside world

```

```

*1 py 0 $ x-z plane, reflective
17 cz 29.135
19 pz 31.75 $ top of reactor
29 pz -31.75 $ bottom of reactor
58 c/z 3.4414 .8515 .3240
268 c/z 3.4414 .8515 .3345
478 c/z 3.4414 .8515 .3475
698 c/z 3.4414 .8515 .4318
880 cz 1.7251
881 cz 1.8051
882 cz 1.9051
905 cz 2.1055
906 c/z 16.7113 0 2.1055
907 c/z -16.7113 0 2.1055
913 c/z 0 11.9185 2.1055
914 c/z 10.3217 5.9592 2.1055
915 c/z 8.3557 14.4724 2.1055
916 c/z -8.3557 14.4724 2.1055
917 c/z -10.3217 5.9592 2.1055
301 px 3.9330
302 px 2.9498
303 p 1 1.7320508076 0 5.8994
304 p 1 1.7320508076 0 3.9330
305 p -1 1.7320508076 0 -9.9834
306 p -1 1.7320508076 0 -2.9498

```

```

imp:n 1 18r 0
m2 92235.50d -.70573 92238.40c -.23821 7014.50d -.05605
m6 41093.40c -1.00000
m7 74000.55d -.74000
m11 5010.03d -.6870 5011.40c -.0840 6012.40c -.2290
m12 1001.60c 1 1002.60c 3 8016.40c 1
mt12 hwtr.01 lwtr.01
pert1:n cell=42,141,40,149 rho=-1.50
kcode 200 .05 5 6
ksrc 3 .2 .2 .2 3 .2 -3 .2 .2 3 .2 4 3 .2 -4 3 .2 4 3 .1 -4 3 .2
e .01 .1 1. 10.

```

```
fq  fe
fc4  fuel rod flux in 5 y locations averaged over 5 x elements
f4:n (154<(42[-10:-6 -1 0])) $ average 5 x elements at j=-1
(154<(42[-10:-6 3 0])) & $ average 5 x elements at j=3
(154<(42[-10:-6 10 0])) $ average 5 x elements at j=10 &
(154<(42[-10:-6 21 0])) $ average 5 x elements at j=21
(154<(42[-10:-6 29 0])) $ average 5 x elements at j=29
sd4  104.7089062 4r      $ 5 times the volume of cell 154
fm4 (1 2 -5) (1 2 -6) (1 2 -7) (1 2 -8) (1 2 4001) (1 2 102021)
→ fc14  fuel rod flux in 5 y locations averaged over 5 x elements
→ f14:n (154<(42[-10:-6 -1 0])) $ average 5 x elements at j=-1
→ (154<(42[-10:-6 3 0])) & $ average 5 x elements at j=3
→ (154<(42[-10:-6 10 0])) $ average 5 x elements at j=10 &
→ (154<(42[-10:-6 21 0])) $ average 5 x elements at j=21
→ (154<(42[-10:-6 29 0])) $ average 5 x elements at j=29
→ sd14  104.7089062 4r      $ 5 times the volume of cell 154
→ fm14 (-1 2 -5) (-1 2 -6) (-1 2 -7) (-1 2 -8) (-1 2 4001) (-1 2 102021)
print 30 90 102 110 160 161 162
prdmp 2j -1
ptrac buffer=20 file=asc write=all event=bnk
```

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