



Knolls Atomic Power Laboratory

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Carlo Code**

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The Physical Models and Statistical Procedures Used in the RACER Monte Carlo Code

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1. INTRODUCTION

This report describes the MCV (Monte Carlo - Vectorized) Monte Carlo neutron transport code [Brown, 1982, 1983; Brown and Mendelson, 1984a]. MCV is a module in the RACER system of codes that is used for Monte Carlo reactor physics analysis. The MCV module contains all of the neutron transport and statistical analysis functions of the system, while other modules perform various input-related functions such as geometry description, material assignment, output edit specification, etc. MCV is very closely related to the O5R neutron Monte Carlo code [Irving *et al.*, 1965] developed at Oak Ridge National Laboratory. O5R evolved into the O5RR module of the STEMB system, which was the forerunner of the RACER system. Much of the overall logic and physics treatment of O5RR has been retained and, indeed, the original verification of MCV was achieved through comparison with STEMB results.

MCV has been designed to be very computationally efficient [Brown, 1981, Brown and Martin, 1984b; Brown, 1986]. It was originally programmed to make use of vector-computing architectures such as those of the CDC Cyber-205 and Cray X-MP. MCV was the first full-scale production Monte Carlo code to effectively utilize vector-processing capabilities. Subsequently, MCV was modified to utilize both distributed-memory [Sutton and Brown, 1994] and shared memory parallelism. The code has been compiled and run on platforms ranging from 32-bit UNIX workstations to clusters of 64-bit vector-parallel supercomputers. The computational efficiency of the code allows the analyst to perform calculations using many more neutron histories than is practical with most other Monte Carlo codes, thereby yielding results with smaller statistical uncertainties. MCV also utilizes variance reduction techniques such as survival biasing, splitting, and rouletting to permit additional reduction in uncertainties.

While a general-purpose neutron Monte Carlo code, MCV is optimized for reactor physics calculations. It has the capability of performing iterated-source (criticality), multiplied-fixed-source, and fixed-source calculations. MCV uses a highly detailed continuous-energy (as opposed to multigroup) representation of neutron histories and cross section data. The spatial modeling is fully three-dimensional (3-D), and any geometrical region that can be described by quadric surfaces may be represented. The primary results are region-wise reaction rates, neutron production rates, slowing-down-densities, fluxes, leakages, and when appropriate the eigenvalue or multiplication factor. Region-wise nuclidic reaction rates are also computed, which may then be used by other modules in the system to determine time-dependent nuclide inventories so that RACER can perform depletion calculations. Furthermore, derived quantities such as ratios and sums of primary quantities and/or other derived quantities may also be calculated. MCV performs statistical analyses on output quantities, computing estimates of the 95% confidence intervals as well as indicators as to the reliability of these estimates.

The remainder of this chapter provides an overview of the MCV algorithm. The following three chapters describe the MCV mathematical, physical, and statistical treatments in more detail. Specifically, Chapter 2 discusses topics related to tracking the histories including: geometry modeling, how histories are moved through the geometry, and variance reduction techniques related to the tracking process. Chapter 3 describes the nuclear data and physical models employed by MCV. Chapter 4 discusses the tallies, statistical analyses, and edits. Chapter 5 provides some guidance as to how to run the code, and Chapter 6 is a list of the code input options.

Overview of the MCV Algorithm

It is assumed that the reader has a fundamental knowledge of the Monte Carlo method for solving the neutron transport equation. For an introduction to this topic, see Chapter 7 of the text by Lewis and Miller (1993). The essential feature of the Monte Carlo method is the simulation of the sequence of events that happens to a neutron in a nuclear system, such as a reactor core. The sequence of events for a single neutron is referred to as a neutron *history*. The history is the basic unit of a Monte Carlo calculation. Quantities such as the energy of a neutron produced by fission, the distance between collisions of the neutron with the nuclei comprising the medium in which it is traveling, etc., are sampled from distribution functions using pseudorandom numbers generated by the code. During the course of a neutron history, the relative likelihood of the various possible events that could occur are used to generate estimates—called *tallies*—of quantities such as reaction rates that are of interest to the user. Since the tallies generated by one history reflect only one particular sequence of events, it is necessary to analyze a large number of histories and average their estimates to obtain meaningful results.

The total number of neutron histories to be analyzed in a calculation is divided into *batches*. The tracking calculations are performed for the histories one batch at a time. This division of the histories into batches has several purposes, but the primary one is that for iterated-source and multiplied-fixed-source calculations the division into batches is the basis for the use of the power method to converge the source. These calculations begin with an initial assumed source distribution for the first batch. The source distribution resulting from fission events caused by the histories of the first batch is used to select the starting locations for the histories for the second batch, and so forth. Eventually, this process converges to the correct source distribution. An additional benefit of the batch-wise algorithm is that computer-memory storage requirements are less than if all histories were tracked simultaneously, but yet computational efficiency is far better than if the histories were analyzed individually. Furthermore, tallies—such as reaction rates—may be determined for each batch and then averaged to yield the final results, and the variation of the tally data from batch to batch may be used to estimate the statistical uncertainty on the final results.

For the purposes of tracking the histories within a batch, the neutron energy range is divided into an arbitrary number of *supergroups*. This is done to control the amount of memory required to hold the cross section data, as only the data required for the energy range corresponding to the current supergroup need to be in memory. The histories are tracked one supergroup at a time starting with the highest-energy supergroup. Those histories with energies in the current supergroup are tracked until all have left the supergroup by virtue of having changed energy or having been terminated, at which point the next-lower-energy supergroup is analyzed (upscattering between supergroups is not permitted in MCV). This process continues until all histories in the batch have been terminated. For the purposes of tallying results, supergroups are combined into *edit groups*. Results are tallied and reported on an edit-group basis. An edit group consists of one or more supergroups that are contiguous in energy. At the highest level the MCV algorithm may be viewed as a set of nested loops, with the outer loop being over the batches. Inside of this loop is the loop over edit groups, which itself contains a loop over those supergroups comprising the current edit group.

A batch begins with the neutron histories originating from source sites with an initial *weight*. The weight in this sense is the relative amount by which a history will contribute to the results of the calculation. In many applications, all histories are assigned an initial weight of unity; in others, one may wish to vary the initial weights based on some problem-specific criteria. The histories are also initially assigned energies based on the characteristics of the neutron source, and directions of motion based on an isotropic distribution. The histories are then tracked through the model geometry until they undergo a collision or escape through the problem boundary. Neutron histories are not terminated by absorption. Upon colliding, the weight is adjusted by multiplying the pre-collision weight by the probability of not being absorbed at the collision point. A collision analysis is then performed to determine the energy and direction of the history following the collision. Histories are terminated by escape through the problem boundary or by a probabilistic method called Russian roulette. In this method, histories are terminated with a probability that depends on their weight in such a manner that low-weight histories have a greater chance of being terminated than high-weight histories. Histories that survive rouletting have their weights increased by a factor that preserves the expected value of the weight before and after rouletting, thus preventing a bias in the results of the calculation. Between the source and terminating events, histories alternate between the tracking and collision analysis phases. Results may be tallied during both of the phases. For calculations involving a fissionable material, fission sites for the next generation may also be generated during the collision phase. The next two chapters describe these phases in more detail.

2. GEOMETRY, TRACKING, AND MATERIAL ASSIGNMENT

There are two primary types of activity involved in following a neutron history from the point at which it is initiated by a source event to the point at which it is terminated. One, collision analysis, refers to the determination of the outcome of a collision event. This topic is discussed in Chapter 3. The other activity, tracking, refers to the mechanism by which the neutron is propagated through the model geometry between collision events. This is the topic of the current chapter.

Section 2.1 describes the two-level geometry representation used in MCV. At the higher level, 3-D space is divided into *sectors*. Sectors may contain a uniform material or they may contain 2-D heterogeneities described by the lower-level geometry representation. Two tracking schemes are available in the code. The first, called *regular tracking*, tracks neutrons from surface to surface until a collision event occurs, at which time the collision is analyzed. The probability of a collision per unit distance traveled is given by the reciprocal of the mean free path (mfp) of the material through which the neutron is moving. Following the collision analysis, tracking is resumed at the post-collision energy and direction of motion. In the second scheme, called *delta or hole tracking*, neutrons are tracked ignoring region boundaries and using a lower bound on the mfp rather than the actual mfp until they suffer a *pseudocollision*. The pseudocollision is then accepted as an actual collision with a probability given by ratio of the lower-bound mfp to the actual mfp. If the collision is accepted, a collision analysis is performed and then the delta tracking resumed. If the collision is rejected, the neutron continues on with no change in energy or angle. This method has the potential to be more efficient than regular tracking in some instances. Section 2.2 discusses regular tracking through a sector composed of a uniform material. This is followed in Section 2.3 by a discussion of regular tracking through a sector that contains 2-D heterogeneities described by the lower level geometry representation. Delta tracking is presented in more detail in Section 2.4. Section 2.5 describes the mechanism used for analyzing sector boundary crossings. The rouletting and splitting techniques for variance reduction are discussed in Section 2.6. How materials are assigned to geometrical regions is the topic of Section 2.7.

2.1 GEOMETRY REPRESENTATION

The basic geometric subdivision used by MCV is referred to as a sector. These three-dimensional volumes must completely fill the model space without overlapping. Sectors are defined in terms of their bounding surfaces. Each surface is specified by a quadratic polynomial of the form

$$F(x, y, z) = a_1x^2 + a_2y^2 + a_3z^2 + a_4xy + a_5yz + a_6zx + a_7x + a_8y + a_9z + a_{10}, \quad (2-1)$$

where (x, y, z) are the Cartesian coordinates of a point in space. The surface is the set of points for which $F(x, y, z) = 0$. The set of points for which F evaluates to a positive number is referred to as the positive side of the surface, and conversely for the negative side. A sector is defined as the intersection of a number of sides. This is accomplished in the code by specifying a list of bounding surfaces and respective senses for each sector, where the sense with respect to a surface indicates whether the sector is on the positive or negative side. For computational efficiency, special forms of Eq. (2-1) are provided for common surfaces such as planes, cylinders, spheres, etc.

A sector may contain either a single uniform material or an embedded *grid*, which is a 2-D geometry representation imposed within a sector. A sector may contain a grid only if the sector is a parallelepiped. The extent of the grid must match the 'base' and 'top' of the parallelepiped exactly, and no variation in composition or geometry is permitted in the direction parallel to the other sides. A sector containing a grid need not be parallel to any particular axis. A grid is defined by a 2-D mesh of parallelograms, which need not be rectangular. Each mesh box within the grid may

further contain arbitrary types and numbers of 2-D quadratic surfaces, limited only by the condition that the quadratic surfaces do not intersect within the mesh box in which they are defined. Quadratic surfaces within a grid do not extend outside the mesh box in which they are defined. Separate, uniform materials may be specified for each mesh box as well as for each region that either lies between two quadratic surfaces or inside a single quadratic surface.

Grids are defined in terms of local, relative coordinate systems, which may differ from the absolute coordinates used for the sector geometry description. On the entry of a neutron into a grid, a 3-D linear transformation is applied to the position and direction coordinates to transform them into the local system. This transformation may include rotation, translation, and scaling of each direction independently. Upon leaving a grid, the inverse transformation is applied to return to the absolute coordinate system of the model. Within a mesh box, another level of translation (but not rotation or scaling) is permitted for the quadratic surfaces. This permits the defining of one set of nested quadratic surfaces to be used in many different mesh boxes, and can result in a very compact description of a problem containing repeated arrays of geometric elements.

Two advantages arise from using grids to describe detailed 2-D geometry. First, the geometry specifications are more compact than for an all-sector description, thus permitting more complex geometries to be represented in a given amount of computer memory. Second, tracking calculations performed by MCV are two to four times faster for grids than for sectors due to the more restrictive geometry specifications of the former.

2.2 TRACKING THROUGH A UNIFORM SECTOR

When a neutron first enters a sector, or as the result of a collision event obtains a new direction of motion within a sector, the distance to the sector boundary along the direction of motion, s , is computed. In addition, a distance to collision, d , is randomly sampled using an exponential distribution based on the mfp of the material in the current region at the neutron energy, i.e.,

$$d = -\lambda_S(E) \ln(\xi), \quad (2-2)$$

where $\lambda_S(E)$ is the mfp for sector S at energy E and ξ is a random number drawn on the interval (0,1). The actual track-length for the neutron is determined using $t = \min(s, d)$, and the neutron is propagated from its original position \mathbf{r}_0 to a new position given by $\mathbf{r} = \mathbf{r}_0 + t \hat{\Omega}$, where $\hat{\Omega}$ is the unit vector in the direction of neutron motion. If $d > s$ then the neutron should now be on the boundary of the sector heading out, and so the boundary crossing routines are called to determine what happens next. If $d < s$ then the neutron has collided at the new position within the same sector, and thus the collision analysis routine is called.

The most complex part of this process is determining the distance to the sector boundary along the direction of motion. Let $F_j(x, y, z) = 0$ denote the equation for surface j bounding the sector of interest. The components of \mathbf{r}_0 and $\hat{\Omega}$ are given by (x_0, y_0, z_0) and (u, v, w) , respectively. Calculation of the distance to this surface, s_j , involves finding the smallest positive root of

$$G_j(s_j) \equiv F_j(x_0 + us_j, y_0 + vs_j, z_0 + ws_j) = 0. \quad (2-3)$$

Equation (2-3) may be recast as

$$G_j(0) + \int_0^{s_j} \frac{d}{ds'} G_j(s') ds' = 0. \quad (2-4)$$

Since $F_j(x, y, z)$ is a quadratic equation, Eq. (2-4) can be solved analytically for s_j . This is done by rewriting Eq. (2-4) one more time taking advantage of the fact that G_j is a quadratic function

$$G_j(0) + \left[\frac{d}{ds'} G_j(s') \right]_{s'=0} s_j + \left[\frac{1}{2} \frac{d^2}{ds'^2} G_j(s') \right]_{s'=0} s_j^2 = 0. \quad (2-5)$$

The coefficients $G_j(0)$, $\left. \frac{d}{ds'} G_j(s') \right|_{s'=0}$, and $\left. \frac{1}{2} \frac{d^2}{ds'^2} G_j(s') \right|_{s'=0}$ are determined, and Eq. (2-5) solved using the quadratic formula for s_j .

The distance to the sector boundary is the smallest positive root (negative roots correspond to the distance in the direction opposite the direction of motion). If no positive root is found, then the neutron will not intersect that surface if it continues in its present direction, and so s_j is set to ∞ . This process is repeated for all surfaces that bound the current sector, and the distance to the sector boundary determined as the minimum value of s_j computed for that sector.

2.3 TRACKING THROUGH A SECTOR CONTAINING A GRID

Surfaces within a sector containing a grid are described by 2-D quadratic polynomials of the form

$$f(x, y, z) = b_1 x^2 + b_2 y^2 + b_3 xy + b_4 x + b_5 y + b_6. \quad (2-6)$$

Grid geometry is uniform in the direction perpendicular to the x - y plane in the local coordinate system of the grid. Distance-to-surface calculations are performed analogously to those for the surfaces bounding the sector, except that they are simplified due to the 2-D nature of the geometry.

Upon entering a sector containing a grid or subsequent to collision event, the distance to the sector boundary along the direction of motion, s , and the distance to collision in the current material, d , are computed as described in Section 2.1 above. Next, the code determines the distance l along the direction of motion to the next grid box boundary or quadric surface within a box. The neutron is propagated from its original position \mathbf{r}_0 to the new position $\mathbf{r} = \mathbf{r}_0 + t \hat{\Omega}$, where t is the smallest of s , d , and l . If d is the smallest of the three values, a collision analysis is performed at the new position and the grid tracking process repeated for the new direction and energy. If l is the smallest value, the tracking process is resumed by determining the distance to collision in the material of the new region and the distance to the next grid box boundary or grid region surface. The distance to the sector boundary is determined by reducing the previous value by the distance just traveled. If d is the smallest value, then the sector boundary crossing routines are called and the identity of the next sector entered is determined.

2.4 DELTA TRACKING

In delta tracking, a lower bound on the neutron mfp is used to determine the distance to the next collision rather than the actual mfp of the material in which the neutron is located. There are two options for determining the lower-bound, or minimum, mfp. As will be discussed in Chapter 3, supergroups in the fast range are divided into small intervals called *subgroups*. In one implementation of the delta tracking scheme, the mfp used for a neutron with energy E is the minimum within the subgroup containing E for all regions within the sector in which the neutron is located. To reduce

computer storage, an alternative scheme determines the minimum mfp over the supergroup containing the neutron energy rather than the subgroup.

In either case, when a neutron enters a sector, or as a result of a collision starts moving in a new direction, the distance to the sector boundary is computed as described in Sections 2.2 and 2.3 above. The distance moved is determined by $t = \min(s, \hat{d})$, where \hat{d} is the sampled distance-to-collision based on the minimum mfp. Note that no calculations to grid box boundaries or grid region surfaces are performed if there is an embedded grid geometry. Since the distance-to-collision calculations are not performed using the physical value for the mfp, these collisions are referred to as pseudocollisions. A pseudocollision is treated as an actual collision with probability \hat{d}/d . This is done by computing a pseudorandom number, and if it is greater than \hat{d}/d the pseudocollision is rejected and tracking is resumed without a change in direction or energy. If, on the other hand, the pseudocollision is accepted the normal collision analysis is performed. A complication is that to perform the collision analysis, the material in which the collision occurred must be known. For the case of grid geometry this must be determined at the time the collision is analyzed, since grid-region-boundary crossings are not determined during the delta tracking process. The location of the neutron in the grid geometry is determined by a binary table search on the indices of the grid boxes. For grid boxes containing quadratic surfaces, further operations are carried out to determine the subregion within the box.

The two neutron tracking schemes available in MCV each have advantages in certain physical situations encountered in applications. The regular scheme is the most effective in sectors that do not contain an embedded grid. It is also the most effective in sectors that contain a grid and in which the neutron mean free path is smaller than the typical linear dimension of the geometric regions within the sector. In this case, most collisions occur in a neutron's current region or in nearby regions, so that relatively few distance calculations are needed per collision. In practical problems, this situation arises in the thermal neutron energy range where mean free paths are smaller. Conversely, fast neutrons have large mean free paths, and many distance calculations and boundary crossings will be performed for each collision. Regular tracking for this case is relatively slow for fast neutrons.

The delta tracking scheme is most effective when the macroscopic total cross-sections in all problem materials are similar, so that the minimum mean free path is relatively close to the actual mean free path. In this case, the fraction of pseudocollisions rejected will be small and excessive table searching will be avoided. In practical problems, this situation arises in the fast neutron energy range, particularly at energies above the resonance range. Conversely, in the thermal and (possibly) resonance energy ranges, the presence of highly concentrated localized absorbers may result in a minimum mean free path which is drastically smaller than "average", and excessive overhead from rejected collisions may result. For these situations, delta tracking may be relatively slow.

From these discussions, it may be inferred that a mixed tracking scheme that uses delta tracking for certain neutron energy ranges and regular tracking for others may have distinct advantages over the individual schemes. Numerical experiments performed in the development of MCV verified this and led to an approach by which the tracking scheme is user-selectable by edit group. The specification of tracking scheme by edit group is necessary for consistency in the tallying of estimators, since these are accumulated for edit groups rather than for individual supergroups. (As will be discussed in Chapter 5, regular tracking provides both path-length and collision estimators, whereas delta tracking provides only pseudocollision estimators.) Different tracking schemes may be used, however, for different edit groups.

2.5 BOUNDARY CROSSINGS

A boundary condition is associated with each side of each sector in a model. Whenever the flight of a history would cause it to cross a surface, the neutron is first stopped at the surface. At this point, an action corresponding to reflection, rotation about a periodicity point, leakage from the model boundary, or unaltered flight into the next sector is then taken based on the boundary condition for the side being left.

A side of a sector may have one or more neighboring sectors. After a neutron leaves a side, undergoes the required boundary operations, and exits a sector, the code must then determine the identity of the new sector being entered. At the start of a calculation, the neighbors of a side are unknown, so that a search must be performed to determine which one has been entered. To this end, MCV is supplied (by another module in the RACER system) with lists

of all of the neighbors on both the positive and negative sides of every surface. The appropriate list is checked, one neighbor at a time, until the new sector is identified. This procedure is costly, however, since many of the neighbors in the list will correspond to sides of sectors other than the one containing the particle. Consequently, the identities of up to four neighbors may be saved for each side of every sector. These neighbors are saved as they are identified during the tracking process. There is thus a two-level neighbor search scheme—the saved-neighbor list for the particular sector and surface is checked first, and only if the correct neighbor is not found there is the exhaustive search performed on the surface neighbor lists for the entire model.

Occasionally, the identity of the new sector cannot be determined. The most frequent cause of this is a modeling error that leaves some portion of the model space unfilled. On extremely rare occasions it may occur as a result of round-off error in the tracking or geometry algorithms. In either case, the history is immediately terminated and this fact noted in the output as a 'lost neutron'. While always undesirable, lost neutrons do not cause a significant problem as long as they represent a negligible fraction of the histories.

For typical models, the frequency of lost neutrons due to round-off is less than one in 10^7 histories. Often, the lost neutron is one that is heading almost directly for an edge formed by the intersection of two sides of a sector. As discussed earlier in this section, RACER first computes which of the two sides the neutron will intercept as well as the distance to the interception point. In the event that the neutron does not collide before reaching the boundary of the sector, it is then moved the computed distance along its direction of motion. Due to round-off, however, the new location of the neutron may result in it intercepting the other of the two sides forming the edge. The inconsistency between the geometry that the code 'thinks' the neutron has moved into and the actual geometry that it now finds the neutron in results in the 'lost' condition.

Certain atypical models have produced lost neutron rates as high as one in 10^5 . These models usually involve complex geometries in which there are instances of three or more surfaces that are meant to intersect along the same line, but due to round-off in the geometry processing instead intersect in pair-wise fashion along multiple closely-spaced lines. The small superfluous volume(s) created by this imperfect geometry representation are 'holes' in the geometry that are unknown to the code. A neutron entering such a hole becomes lost.

2.6 ROULETTING AND SPLITTING

Rouletting and splitting [Carter and Cashwell, 1975; Lewis and Miller, 1993] are complementary techniques used to maximize the efficiency of the Monte Carlo calculation. These methods are used to maximize the fraction of the computational effort devoted to tracking histories that contribute most to reducing the uncertainty of the desired results. Both are implemented in MCV using user-specified position- and energy-dependent minimum, nominal, and maximum weight standards—denoted by w_{\min} , w_{nom} , and w_{\max} , respectively—where $w_{\min} \leq w_{\text{nom}} \leq w_{\max}$. When a neutron crosses a region boundary or emerges from a collision, its weight is compared to the minimum and maximum weight standards for the current region and energy range. If the weight is less than the minimum, then rouletting is performed; if the weight is greater than the maximum, then splitting is performed; otherwise, the neutron proceeds on as normal. In rouletting, a history with weight w less than w_{\min} is terminated with probability $1 - (w/w_{\text{nom}})$. If the history is not terminated, then the weight is increased to w_{nom} . In splitting, a history with weight greater than w_{\max} is split into multiple histories of weight w_{nom} each. With probability $(w/w_{\text{nom}}) - \lfloor w/w_{\text{nom}} \rfloor$ (the operator ' $\lfloor \dots \rfloor$ ' indicates that the integer part is to be taken) the original history is split into $\lfloor w/w_{\text{nom}} \rfloor + 1$ histories; otherwise, it is split into $\lfloor w/w_{\text{nom}} \rfloor$ histories. Both rouletting and splitting conserve the expected value of the weight.

2.7 MATERIAL ASSIGNMENT

A fundamental concept in the description of a RACER Monte Carlo model is that of an *edit medium*. An edit medium may be thought of as the union of a set of geometrical regions that need not be contiguous. Results in RACER are either reported for the model as a whole, or are broken down spatially based on edit media. A geometrical region that comprises part of an edit medium may be an entire uniform sector, or it may be a region of the grid geometry contained within a sector.

Another important concept is that of a *material*. In RACER terminology, a material is a homogeneous mixture, the composition of which is specified by the number densities of its constituent nuclides. In addition to providing the geometrical specification of the volume over which results are tallied, edit media serve the dual function as the mechanism by which materials are assigned to the spatial regions. Normally, each edit medium must consist of a single material. Thus, nuclides are assigned to materials, materials are assigned to edit media, and edit media are assigned to geometrical regions. The exception to the one-material-per-edit-medium rule is through the use of an *axially-varying-composition* feature (called AXCOMP in RACER jargon). Using this feature, the material assignment for an edit medium is allowed to vary discontinuously only in the axial direction. The axial direction referred to here is that of the local coordinate system within a sector.

3. NUCLEAR DATA AND PHYSICS MODELS

An important feature of the MCV code is its highly detailed representation of neutron cross sections and treatment of neutron-nucleus interaction physics. The neutron energy spectrum is divided into two ranges, the fast range and the thermal range. The energy that divides these two ranges—referred to as the thermal cutoff—is variable, but is typically set at 0.625 eV. Since different physical effects dominate at high and low energies, the neutron cross section representation and physics treatments differ between the two energy ranges. Neutron energy is always treated as a continuous variable in the fast range. Both continuous-energy and multigroup options are available in the thermal range. In Section 3.1 descriptions of the various nuclear data representations are provided. Section 3.2 discusses the neutron-nucleus interaction models used.

3.1 NUCLEAR DATA

With two exceptions nuclear interaction data are supplied to the RACER system by a system of codes referred to as NTOA. This system includes the widely-used NJOY code [MacFarlane, *et al.*, 1982] for processing ENDF nuclear data files [McLane, *et al.*, 1990]. The exceptions are the probability tables for treating the unresolved resonance range (URR), which are generated from the ENDF/B data by other codes; and the data used for the continuous-energy thermal range treatment, which is obtained by the RACER system directly from the ENDF/B files.

3.1.1 Fast-Range Cross Sections

As discussed in Chapter 1, the neutron energy range is divided into an arbitrary number of divisions called supergroups. The fast range consists of one or more supergroups with energy boundaries chosen based on variations in physical data. Each supergroup is then divided into subgroups of equal energy width. Cross sections are tabulated at subgroup midpoints and are assumed to vary as $1/v$ within each subgroup. Typical calculations utilize 166 fast-range supergroups having 128 subgroups each, for a total of 21,248 subgroups.

In addition to the total cross section, MCV utilizes the elastic scattering, inelastic scattering, fission, and v -fission cross sections. The capture cross section is obtained implicitly by subtracting the scattering and fission cross sections from the total. In actuality, what the RACER system refers to as the 'inelastic scattering' cross section consists of the sum of the true inelastic scattering, $(n,2n)$, and $(n,3n)$ cross sections. The reason for this is that the secondary neutrons produced by all of these mechanisms are treated identically in the code, as will be described further on. The ' v -fission' cross section is simply the product of the fission cross section and v , the mean number of neutrons produced per fission. This quantity is tabulated separately from the fission cross section since v will in general vary with energy. The fast cross sections are supplied to the RACER system by NTOA in a format called EVDF (*E*Valuated *D*ata *F*iles), in which cross section variation as a function of energy is represented by cross section values tabulated at discrete energy points. The number and energies of the tabulated points vary from nuclide to nuclide, and from cross-section-type to cross-section-type for a particular nuclide. Preprocessing modules in the RACER system construct job-dependent cross section libraries in which all cross sections are tabulated at the subgroup midpoints for all nuclides and cross-section-types. The tabulated cross sections are obtained by lethargy-averaging the EVDF cross sections over the subgroup. This procedure preserves the infinitely-dilute resonance integral for the subgroup, which means that broader subgroups may be used than would have been possible had the subgroup midpoint values simply been obtained by interpolating the EVDF data.

3.1.2 Scattering Angle Distributions for Elastic Scattering

The default treatment of elastic scattering from all nuclides with the exception of ^1H bound in water is through the use of target-at-rest kinematics and the sampling of the cosine of the scattering angle in the center-of-mass (COM) system (μ_c) from a distribution function parameterized by the neutron energy. These distribution functions are represented in MCV using step functions with equally-probable steps. The number of steps is user-selectable, with 31 being a typical value. These distribution functions are created within the RACER system from Legendre moments of the COM scattering cosine distributions supplied by NTOA.

There are two special cases that do not follow the above prescription. For nuclides that scatter isotropically, only one step function with bounds of $\mu_c = -1$ and $\mu_c = 1$ is used for all energies within the supergroup. For nuclides treated as linearly anisotropic scatterers, a single step is used at each energy subinterval within the supergroup. For nuclides for which the first Legendre moment (P_1) is positive, the step is non-zero over the range $2P_1 - 1 < \mu_c \leq 1$; for those with a negative first moment, the step is non-zero over the range $-1 \leq \mu_c < 2P_1 + 1$. These choices of the step bounds ensure that the average center-of-mass scattering angle is preserved.

For nuclides other than ^1H , an optional 'effective- α ' method (described in Section 3.2.2) is available for treating elastic scattering. The use of this method only affects the calculation of the scattered neutron energy, however. The scattering angle calculation is still performed using the standard target-at-rest kinematics.

3.1.3 Inelastic/(n,xn) Transfer Matrices

As will be discussed later in this chapter, MCV treats inelastic scattering, (n,2n), and (n,3n) reactions using multi-group transfer matrices provided by NTOA. The 25 highest-energy MUFT [Bohl, *et al.*, 1957] groups (those above 5.531 keV, with the top group extended to 20 MeV) are used for defining the matrix elements, which give the mean number of secondary neutrons produced in each exit MUFT group due to an inelastic scattering, (n,2n), or (n,3n) event in the same or another MUFT group.

3.1.4 Probability Tables for the Unresolved Resonance Range

MCV has an optional capability to use probability tables to obtain cross section values in the unresolved range. These tables are tabulated at a predetermined set of energy points and temperatures. Tables at different temperatures are properly correlated. The number of cross section bands, energy points, and temperatures are variable; but typical usage is ten bands, one energy point per supergroup that lies within the URR, and nine temperatures. The probability tables are computed by the PROTAB and CONTAB codes [Sutton and Brown, 1998].

3.1.5 Multigroup Thermal Range Cross Sections and Transfer Matrices

The thermal energy range consists of a single supergroup, and utilizes one of two possible cross section treatments. In the multigroup treatment, multigroup cross sections and transfer matrices obtained from NTOA are used. The transfer matrices contain the probabilities of scattering from one thermal group to another, and the first Legendre moments of the associated laboratory-system scattering cosines. The transfer matrices are only supplied for certain nuclides designated as 'moderators'. Typical calculations employing this treatment use 32 energy subgroups in the thermal supergroup.

3.1.6 Continuous-Energy Thermal Cross Sections

A newer and more accurate method allows for a continuous-energy treatment of neutron histories and nuclear data in the thermal range. The required nuclear data are obtained, when available, directly from the ENDF/B files.

3.1.7 Source Spectra

The ENDF/B-VI ^{235}U combined prompt and delayed thermal fission spectrum is coded directly into MCV in the form of a piecewise-linear, discontinuous function having 1031 line segments. MCV also contains routines to sample prompt and delayed neutrons from Watt and Maxwellian spectra, respectively, where the spectral parameters are appropriate to ^{235}U . Other spectra may be supplied by the user through the RACER system input modules.

3.1.8 Doppler Broadening

MCV has the capability to Doppler broaden cross section data from the temperature at which it is provided to the calculation to any higher temperature. The implementation of this in-line Doppler broadening algorithm is identical to that found in the BROADR routine of NJOY [MacFarlane, 1989], which is itself based on the "kernel broadening" method used in the SIGMA1 code [Cullen, 1978]. A full description of this method can be found in the NJOY manual.

The MCV implementation broadens the cross section data from the temperatures at which they are provided (the *reference temperatures*) to *target temperatures* provided by the user. Cross section libraries are typically created at two reference temperatures designated as "hot" and "cold". The target temperatures may be specified individually for each composition in the model. When Doppler broadening moderators, MCV utilizes an effective temperature rather than the actual temperature to account for the kinetic energy of the bound nuclei. Effective temperatures corresponding to both the target and reference temperatures are determined, and the difference between these are then used to broaden the cross section data.

3.2 PHYSICS MODELS

3.2.1 The Neutron Source

Sampling the Source Site Locations

Three methods are employed to select the initial locations for the histories within a batch. In the first of these, one or more source regions are defined as rectangular boxes with sides perpendicular to the x -, y -, and z -axes. In the simplest version of this method, source locations are randomly assigned to a source region with a probability proportional to the volume of the source region. Within a source region, the source location is sampled from a uniform distribution. An extension to this method allows one to specify that source locations may only be sampled within specified edit media within the source region. When this option is used, source sites are uniformly distributed within the volumes of the specified edit media included within any source region. This method is employed in distributed fixed-source calculations, for the fixed component of the source in multiplied-fixed-source calculations, and for the source for the initial batch in iterated-source calculations.

In the second method the source locations are selected randomly from sites generated in the previous batch. If the number of sites is less than the number of histories needed in the batch, every site is split n -for-1, where n is the smallest integer such that n times the initial number of sites is greater than or equal to the number of histories needed.

The starting locations are then selected randomly from the set of split sites uniformly and without replacement. This method is used for all batches subsequent to the initial batch in iterated-source calculations, and for the iterated component of the source in multiplied-fixed-source calculations.

The third method allows the user to define the locations of a number of point sources. The initial location of the histories are randomly sampled from the set of points, with each point having an equal probability of being sampled.

Sampling the Energy

There are several source spectrum options available. The following are coded into MCV in the form of piecewise-linear discontinuous functions:

- a linear combination of the ENDF/B-VI ^{235}U prompt and delayed fission spectra (β , the delayed neutron fraction, is the combining coefficient),
- a Watt spectrum (sometimes used for prompt fission neutrons),
- a Maxwellian spectrum (sometimes used for delayed fission neutrons),
- a linear combination of Watt and Maxwellian spectra.

There is also the ability to use user-supplied spectra. These may take the form of histograms or a set of discrete energy points and associated probabilities.

Sampling the Direction

All sources are assumed to be isotropic, so initial directions are sampled uniformly over the unit sphere. This is achieved by sampling the cosine of the polar angle uniformly on the interval (-1,1), and the azimuthal angle uniformly on the interval (0,2 π).

3.2.2 Fast-Range Physics

The analysis of fast neutron transport physics includes two distinct phases. In one phase, macroscopic data for a material are used to sample the distance to collision, to determine the history weight modification upon collision, to tally the estimators, and to select a scattering nuclide. In the other phase, data specific to the scattering nuclide are used to determine the exit energy and direction. These procedures are discussed in detail below.

Mean Free Path

For subgroup i of material m , the tabulated mfp is given by

$$\lambda_{i,m} = 1/\Sigma_{t,i,m}, \quad (3-1)$$

where

$$\Sigma_{t,i,m} = \sum_j N_{j,m} \sigma_{t,i,j} \quad (3-2)$$

is the total macroscopic cross section at the energy midpoint of the subgroup, the summation is over all nuclides j in material m , $N_{j,m}$ is the number density of nuclide j in material m , and $\sigma_{t,i,j}$ is the microscopic total cross-section for nuclide j at the energy midpoint of the subgroup. Within subgroup i , the mean free path to collision as a function of neutron energy, E , using the aforementioned $1/v$ interpolation law for cross section data, is thus

$$\lambda_m(E) = \frac{v}{v_i} \lambda_{i,m} \quad (3-3)$$

where v is the neutron speed and v_i is the speed corresponding to the subgroup midpoint.

The mfp given by Eq. (3-3) is used to sample the distance to collision for regular tracking in material m as described in Section 2.2. If delta tracking is used, then the minimum mfp for the sector and delta tracking energy range is used as described in Section 2.4. If delta tracking cross sections are determined by subgroup, then the minimum mfp for a neutron in sector S and subgroup i is given by

$$\lambda_{\min, S, i} = \min_{m \in S} \left[\frac{v_{\text{low}, i}}{v_i} \lambda_{i, m} \right], \quad (3-4)$$

where $v_{\text{low}, i}$ is the neutron speed corresponding to the lowest energy in subgroup i , and the minimum is found over all materials contained in the sector. If delta tracking cross sections are determined by supergroup, then the minimum mfp for sector S and supergroup g is given by

$$\lambda_{\min, S, g} = \min_{\substack{i \in g \\ m \in S}} \left[\frac{v_{\text{low}, i}}{v_i} \lambda_{i, m} \right], \quad (3-5)$$

where the minimum is found over all subgroups in the supergroup as well as over all materials contained in the sector.

Survival Probability

The survival (non-absorption) probability for subgroup i and material m is given by

$$p_{\text{survival}, i, m} = \Sigma_{s, i, m} / \Sigma_{t, i, m} \quad (3-6)$$

where the macroscopic scattering cross-section at the energy midpoint of subgroup i is given by

$$\Sigma_{s, i, m} = \sum_j N_{j, m} \sigma_{s, i, j}, \quad (3-7)$$

and $\sigma_{s, i, j}$ is the microscopic scattering cross-section at the energy midpoint of the subgroup. As the ratio of two macroscopic cross-sections having $1/v$ behavior, p_{survival} is constant within a subgroup. As mentioned in the Introduction, absorption events do not terminate neutron histories in MCV. Rather, given a collision in subgroup i and material m , the neutron weight is multiplied by p_{survival} , so that the correct expected weight emerges from the collision. This process is known as survival biasing [Carter and Cashwell, 1975], and can greatly enhance the efficiency of a Monte Carlo calculation.

Fission Neutron Emission Probability

The fission neutron emission probability is given by

$$p_{v\text{-fission}, i, m} = (v \Sigma_{f, i, m}) / \Sigma_{t, i, m}, \quad (3-8)$$

where the macroscopic ν -fission cross section at the energy midpoint of subgroup i is given by

$$\nu\Sigma_{f,i,m} = \sum_j N_{j,m} \nu\sigma_{f,i,j}, \quad (3-9)$$

and where $\nu\sigma_{f,i,j}$ is the microscopic nu-fission cross section of nuclide j at the energy midpoint of subgroup i . Being a ratio of cross sections, $p_{\nu\text{-fission}}$ is constant within a given subgroup. In iterated-source and multiplied-fixed-source calculations, this quantity is used in selecting potential fission source sites from which the fission source sites for the next generation (batch) are sampled. For each collision within a fissionable material, the quantity

$$p_{\text{site}} = p_{\nu\text{-fission}, i, m} w / \hat{w} \quad (3-10)$$

is determined, and $\lfloor p_{\text{site}} \rfloor$ potential fission source sites are created at the coordinates of the collision. In addition, an additional site is created at these coordinates with probability $p_{\text{site}} - \lfloor p_{\text{site}} \rfloor$. The quantity \hat{w} is used to adjust the expected number of sites that will be generated. The mean number of potential sites produced in a batch is given by kN/\hat{w} , where k is the multiplication factor for the batch and N is the number of histories in the batch. The parameter \hat{w} is set to a value 20 percent less than the current best estimate of the eigenvalue. In this way, on the average 20 percent more sites will be generated than are required for the next batch. This minimizes the likelihood that an insufficient number of sites will be produced—thereby requiring that some sites be used more than once to select the starting locations for the histories in the next batch; or that far too many sites will be produced—thereby requiring that memory be reserved to accommodate them.

Selection of Scattering Nuclide

When a collision occurs for a neutron with energy E moving in direction Ω , a scattering nuclide is sampled for the purposes of determining the exit energy E' and direction Ω' . For a neutron with an incident energy in subgroup i that collides in material m , the probability that nuclide j is sampled is

$$p_{\text{scatter}, i, m, j} = N_{j, m} \sigma_{s, i, j} / \Sigma_{s, i, m}. \quad (3-11)$$

Elastic Scattering Analysis

The initial determinations of the cosine of the scattering angle (μ) and exit energy in the laboratory system for all collisions are based upon elastic scattering with target-at-rest kinematics. Later, these results may be modified to account for scattering from bound hydrogen and for inelastic scattering. Elastic scattering analyses proceed in three steps: first, the cosine of the scattering angle in the COM, μ_c , is sampled from a tabulated probability distribution function (PDF); next, the exit energy and scattering angle cosine in the laboratory system are determined from the kinematics of elastic scattering from a target at rest; and finally, an azimuthal angle is sampled uniformly, and the neutron's direction cosines are updated.

The cosine of the center-of-mass scattering angle is obtained by random sampling from PDFs that represent the angular scattering distribution as equally-probable step functions (i.e., a histogram distribution, with each rectangle having the same area). The use of equally-probable step functions eliminates the possible negativity problems of other methods such as those based on Legendre expansions or discrete angle PDFs at the zeros of a Legendre polynomial. The equally-probable step function PDFs are tabulated for each scattering nuclide at equally-spaced energy intervals within a supergroup. The number of energy intervals need not be the same as the number of subgroups used for tabulating the macroscopic material cross-sections and, indeed, may vary from nuclide to nuclide. The number of steps may also vary between nuclides, but—for a given nuclide—the number of steps is required to be the same at each energy interval within the supergroup. Selection of the COM scattering angle cosine is accomplished via a two

stage sampling procedure: first, one step of the histogram PDF is randomly and uniformly selected; then, the scattering cosine is randomly sampled uniformly within that step.

Given the sampled value μ_c , the laboratory scattering angle cosine and exit energy are determined using [Henry, 1975]

$$\mu = \frac{A\mu_c + 1}{\sqrt{A^2 + 2A\mu_c + 1}} \quad (3-12)$$

and

$$E' = E \frac{A^2 + 2A\mu_c + 1}{(A + 1)^2}, \quad (3-13)$$

where A is the ratio of the target mass to that of the neutron and E is the incident neutron energy in the laboratory system. The azimuthal angle, ϕ , is randomly sampled from a uniform distribution on the interval $(0, 2\pi)$.

The post-collision direction cosines are given by

$$\Omega'_x = \Omega_x \mu - \sqrt{1 - \Omega_x^2} \sqrt{1 - \mu^2} \cos \phi, \quad (3-14a)$$

$$\Omega'_y = \Omega_y \mu + \frac{\sqrt{1 - \mu^2}}{\sqrt{1 - \Omega_x^2}} (\Omega_x \Omega_y \cos \phi - \Omega_z \sin \phi), \quad (3-14b)$$

and

$$\Omega'_z = \Omega_z \mu + \frac{\sqrt{1 - \mu^2}}{\sqrt{1 - \Omega_x^2}} (\Omega_x \Omega_z \cos \phi + \Omega_y \sin \phi); \quad (3-14c)$$

where Ω_u , $u = \{x, y, z\}$, are the pre-collision direction cosines, and the Ω'_u are the post-collision values. For values of $|\Omega_x|$ very close to unity, the following expressions are used due to their greater accuracy in this case:

$$\Omega'_x = \mu, \quad (3-15a)$$

$$\Omega'_y = \sqrt{1 - \mu^2} \cos \phi, \quad (3-15b)$$

and

$$\Omega'_z = \sqrt{1 - \mu^2} \sin \phi. \quad (3-15c)$$

Inelastic Scattering Analysis

Inelastic scattering may be treated as isotropic in either the laboratory or center-of-mass systems, according to user input. In either case, the post-collision directions are determined the same as for elastic scattering. The exit energy,

however, is determined using the inelastic/(n,xn) matrices described in Section 3.1.3. First, the initial MUFT group containing the incident energy is determined. Next, the exit MUFT group is determined using a discrete PDF obtained by normalizing the matrix elements corresponding to the initial MUFT group to unity. If the exit group is different from the initial group, then the exit energy is uniformly sampled within the exit group. If the exit group and the initial group are the same, then the exit energy is uniformly sampled from the energy range extending from the incident energy to the lowest energy of the MUFT group.

As mentioned in Section 3.1.3, the transfer matrices account for (n,2n) and (n,3n) reactions as well as for inelastic scattering. Since the matrix elements are defined as the number of secondary neutrons that appear in the exit group due to an inelastic scattering, (n,2n), or (n,3n) event in the initial group, the sum of matrix elements corresponding to an initial group will be greater than unity if there is an (n,xn) contribution—thus the need for the normalization mentioned in the previous paragraph. To account for neutrons created by (n,xn) reactions, the weight of the history is modified by a multiplier equal to the normalization factor. Thus, new histories are not created by (n,xn) reactions, but rather the weight of the history is increased.

Bound Hydrogen Scattering

Chemical binding effects on hydrogen bound in water molecules are significant for neutron scattering at fast-range energies. The use of proton-at-rest models for fast-range bound-hydrogen scattering can lead to errors in the fast flux and to errors in the thermal-energy-range slowing-in energy and angular distributions. In MCV, a modified free-gas model is used to analyze fast-range bound-hydrogen scattering. In this model, hydrogen bound in water is treated as a gas at an effective temperature, with upscattering replaced by scattering without energy change.

Following Cady, *et al.* [1967], the P_0 component of the proton free-gas differential cross section in the laboratory system is given by

$$\sigma_{H,0}(E \rightarrow E') \equiv \int_{-1}^1 d\mu \sigma_H(E \rightarrow E', \mu) \quad (3-16)$$

$$= \begin{cases} \sigma_{H,0}^u(E \rightarrow E') = \frac{\hat{\sigma}_H}{E} \exp\left(\frac{E-E'}{kT_{\text{eff}}}\right) \text{erf}\left(\sqrt{\frac{E}{kT_{\text{eff}}}}\right), & E' > E \\ \sigma_{H,0}^d(E \rightarrow E') = \frac{\hat{\sigma}_H}{E} \text{erf}\left(\sqrt{\frac{E'}{kT_{\text{eff}}}}\right), & E' < E \end{cases}$$

where $\hat{\sigma}_H$ is the free hydrogen scattering cross section, k is Boltzmann's constant, and T_{eff} is an effective temperature determined from the moderator temperature using the Cady-Nelkin model [Nelkin, 1960]. Since in the fast range the neutron energies are much greater than kT_{eff} , the integrals of the up- and down-scattering differential cross sections over all exit energies may be approximated by

$$\sigma_{H,0}^u(E) = \hat{\sigma}_H \frac{kT_{\text{eff}}}{E} \quad (3-17a)$$

and

$$\sigma_{H,0}^d(E) = \hat{\sigma}_H \left(1 - \frac{kT_{\text{eff}}}{2E}\right). \quad (3-17b)$$

The probability of up-scattering is thus

$$P_{\text{up}} = \frac{\sigma_{\text{H},0}^{\text{u}}(E)}{\sigma_{\text{H},0}^{\text{u}}(E) + \sigma_{\text{H},0}^{\text{d}}(E)} = \frac{kT_{\text{eff}}}{E + kT_{\text{eff}}/2} \quad (3-18)$$

The conditional PDF for the exit energy given that a down-scattering has occurred is

$$f_{\text{free-gas}}(E \rightarrow E') = \frac{\sigma_{\text{H},0}^{\text{d}}(E \rightarrow E')}{\sigma_{\text{H},0}^{\text{d}}(E)} = \frac{\text{erf}\left(\sqrt{\frac{E'}{kT_{\text{eff}}}}\right)}{E - kT_{\text{eff}}/2} \quad (3-19)$$

The exit energy PDF for hydrogen scattering based on target-at-rest kinematics is

$$f_{\text{target-at-rest}}(E \rightarrow E') = 1/E, \quad (3-20)$$

so that the ratio of the free-gas to target-at-rest PDFs is

$$W(E \rightarrow E') = \frac{f_{\text{free-gas}}(E \rightarrow E')}{f_{\text{target-at-rest}}(E \rightarrow E')} = \frac{\text{erf}\left(\sqrt{\frac{E'}{kT_{\text{eff}}}}\right)}{1 - \frac{kT_{\text{eff}}}{2E}} \quad (3-21)$$

The P_1 component of the proton free-gas differential down-scattering cross section in the laboratory system is given by

$$\begin{aligned} \sigma_{\text{H},1}(E \rightarrow E') &\equiv \int_{-1}^1 d\mu \mu \sigma_{\text{H}}(E \rightarrow E', \mu) \quad (3-22) \\ &= \sigma_{\text{H},1}^{\text{d}}(E \rightarrow E') = \frac{\hat{\sigma}_{\text{H}}}{E^{3/2} \sqrt{kT_{\text{eff}}}} \left[\left(\sqrt{\frac{E'}{kT_{\text{eff}}}} - \sqrt{\frac{kT_{\text{eff}}}{E'}} \right) \text{erf}\left(\sqrt{\frac{E'}{kT_{\text{eff}}}}\right) + \frac{2}{\sqrt{\pi}} \exp\left(\frac{-E'}{kT_{\text{eff}}}\right) \right], E' < E \end{aligned}$$

The mean cosine of the scattering angle in the laboratory system for down-scattering from bound hydrogen is thus

$$\bar{\mu}_{\text{H}}(E \rightarrow E') = \frac{E'}{E} \left[1 - \frac{kT_{\text{eff}}}{E'} + \frac{2}{\sqrt{\pi}} \sqrt{\frac{kT_{\text{eff}}}{E'}} \frac{\exp\left(\frac{-E'}{kT_{\text{eff}}}\right)}{\text{erf}\left(\sqrt{\frac{E'}{kT_{\text{eff}}}}\right)} \right] \quad (3-23)$$

The use of Eq. (3-23) causes numerical difficulties for $E'/(kT_{\text{eff}}) \ll 1$. This problem is addressed in MCV by setting the cosine of the laboratory scattering angle to zero when $E'/(kT_{\text{eff}}) < 0.1$. This is judged to have negligible effect on calculational results for two reasons: (1) scattering from energies greater than 0.625 eV directly to energies less than $(0.1 \cdot kT_{\text{eff}})$ will occur infrequently, and (2) the true expected value of the free-gas scattering angle cosine for these cases approaches zero.

Equations (3-18), (3-21), and (3-23) form the basis of the bound hydrogen scattering procedure used in the MCV code. The following steps are performed to analyze collisions at energy E with hydrogen in the fast range:

- Sample the laboratory scattering angle cosine μ and the corresponding exit energy E' using target-at-rest

- kinematics for free hydrogen with isotropic center-of-mass scattering.
- Using p_{up} , randomly determine whether the free gas model yields an exit energy greater than the incident energy.
 - If so, change the scattering cosine to unity and the exit energy to the incident energy (i.e., use a delta scattering approximation).
 - If not, keep the exit energy at the value given by the target-at-rest kinematics analysis, modify the weight of the history by the multiplicative factor $W(E \rightarrow E')$, and change the laboratory scattering cosine to $\bar{\mu}_H$.
 - Randomly sample the azimuthal angle and determine the post-scattering direction cosines.

This procedure gives the correct Cady-Nelkin expected value for the cosine of the scattering angle for free-gas down-scattering, since the expected value is always used as the scattering cosine and random sampling of the cosine is not performed. Furthermore, the correct Cady-Nelkin exit energy distribution of history weight is also preserved. This procedure has been tested both in the MCV code and separately in comparisons with the scalar rejection-sampling scheme used in the STEMB modified free gas kernel. In all comparisons to date, the MCV results are statistically indistinguishable from the results of the STEMB sampling scheme.

Heavy Nuclide Binding Model

MCV will optionally use an "effective- α " model to treat the effects of binding on scattering from all nuclides heavier than ^1H . First, target-at-rest kinematics are used to determine the exit energy $E'_{\text{target-at-rest}}$ and center-of-mass scattering cosine μ_c . If the target-at-rest exit energy is within the fast energy range, then the actual exit energy assigned to the neutron is

$$E' = (1 - \kappa)E + \kappa E'_{\text{target-at-rest}}, \quad (3-24)$$

where

$$\kappa = \frac{1}{1 + (2 - 1/(2A))(kT_\alpha/E)}, \quad (3-25)$$

k is Boltzmann's constant, and T_α is a user-supplied effective temperature. If the target-at-rest exit energy falls within the thermal range, then the exit energy is given by

$$E' = \left[1 - \frac{E_{\text{thermal}} - \alpha E}{E_{\text{thermal}} - \alpha' E} \right] E_{\text{thermal}} + \frac{E_{\text{thermal}} - \alpha E}{E_{\text{thermal}} - \alpha' E} [(1 - \kappa)E + \kappa E'_{\text{target-at-rest}}], \quad (3-26)$$

where E_{thermal} is the energy marking the boundary between the fast and thermal ranges,

$$\alpha = \left(\frac{A - 1}{A + 1} \right)^2, \quad (3-27)$$

and

$$\alpha' = 1 - \kappa(1 - \alpha). \quad (3-28)$$

The post-collision direction cosines are determined using the target-at-rest value of the laboratory-system scattering cosine.

The Unresolved Resonance Range

MCV has two options for dealing with the unresolved resonance range (URR). One option simply utilizes continuous-energy dilute-average cross section data, treating it the same way as cross section data in the rest of the fast range. The more accurate treatment utilizes probability tables to account for the fine-scale variability of the cross sections in the URR. The probability table method [Nikolaev, *et al.*, 1970; Levitt, 1972] divides the range of total cross section values into discrete bands. The probability tables consist of *band-averaged* total and partial cross sections, and the probabilities that the total cross section lies within each band. The tables are generated at a set of discrete incident energies and temperatures. When a neutron undergoes a collision in the URR of a nuclide, the cross section is randomly sampled using the band probabilities of the table for that nuclide at the nearest temperature and energy. The sampled value is then modified by adding an amount equal to the difference between the dilute-average value at the collision energy and the dilute-average value at the table energy [Sutton and Brown, 1998]. This method preserves the continuous-energy dilute-average cross sections while at the same time capturing the effect of the cross section variation due to unresolved resonances.

3.2.3 Multigroup Thermal-Range Physics

The original thermal energy range physics treatment used by MCV is based on a multigroup model and P_1 scattering. Scattering nuclides are classed as moderators or non-moderators. As in the fast-range physics description, macroscopic material data are used in neutron tracking and in selecting the scattering nuclide. Nuclidic scattering data are used in determining the exit neutron direction and energy.

Material Data

The macroscopic quantities computed for each material are the mean free path, the survival probability, and the fission neutron emission probability. These are tabulated for each thermal group and assumed to be constant within the group. For group g of material m :

$$\lambda_{g,m} = 1/\Sigma_{t,g,m}, \quad (3-29)$$

$$P_{\text{survival},g,m} = \Sigma_{s,g,m}/\Sigma_{t,g,m}, \quad (3-30)$$

and

$$P_{\text{v-fission},g,m} = (\nu\Sigma_{f,g,m})/\Sigma_{t,g,m}. \quad (3-31)$$

where the symbols have the same meaning in a group-averaged sense as those defined for the fast-range analysis. As in the fast-range analysis, absorption events are not allowed to terminate neutron histories, and $P_{\text{survival},g,m}$ is used to modify the neutron weights. Similarly, $P_{\text{v-fission},g,m}$ is used in selecting potential fission sites for the next generation in iterated-fission problems. The selection of nuclide j as the scattering nuclide is based on the scattering probability

$$P_{\text{scatter},g,m,j} = N_{j,m}\sigma_{s,i,j}/\Sigma_{s,i,m}. \quad (3-32)$$

Multigroup Scattering Analysis

The scattering analysis differs depending on whether or not the scattering nuclide is classified as a moderator or as a non-moderator. Non-moderators, or 'heavy nuclides', are assumed to have infinite mass—that is, they are assumed to

scatter neutrons isotropically in the laboratory system without altering neutron energy. A laboratory-system scattering cosine is thus uniformly sampled on the interval $(-1,1)$, the azimuthal angle is uniformly sampled on the interval $(0,2\pi)$, and the exit group is the same as the incident group.

If the scattering nuclide is classified as a moderator, the exit group is determined via random sampling from a discrete PDF for scattering from a given initial group to all possible exit groups. Upscattering is allowed in the thermal range, but not to energies greater than the thermal/fast range boundary. Any neutrons that would have scattered to an energy in the fast range are put into the top thermal group. The sampled exit group number is used to obtain the tabulated P_1 component of the laboratory-system scattering angle distribution. The laboratory-system scattering angle is sampled from a single-step distribution function constructed as described in Section 3.1.2 for elastic scattering in the fast range.

3.2.4 Continuous Energy Thermal-Range Physics

MCV provides the user with the option of modeling a neutron transport problem using a continuous energy treatment over the entire energy range. Cross sections are tabulated as histograms with equal-lethargy width bins. The number of bins used to describe the thermal supergroup is specified by the user, with 1000 being a typical value. Three scattering law formalisms [McLane, 1990] are used to treat the three major scattering mechanisms in the thermal range: i.e., incoherent inelastic, coherent elastic, and incoherent elastic. Each of these will be described in turn.

Incoherent Inelastic Scattering

The continuous energy thermal treatment in MCV uses ENDF/B $S(\alpha, \beta)$ scattering law data directly to analyze incoherent inelastic collisions [Ballinger, 1995]. The double differential scattering cross section can be expressed as

$$\sigma_s(E \rightarrow E', \mu, T) = \frac{\left(\frac{A+1}{A}\right)^2 \sigma_{\text{free}}}{2k_B T} \sqrt{\frac{E'}{E}} e^{-\beta/2} S(\alpha, \beta, T), \quad (3-33)$$

where σ_{free} is the free nucleus scattering cross section, A is the ratio of the mass of the target to that of the neutron, T is the moderator temperature, E is the incident energy, E' is the exit energy, μ is the laboratory-system scattering cosine, $S(\alpha, \beta, T)$ is the scattering law,

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{AkT}, \quad (3-34)$$

and

$$\beta = \frac{E' - E}{kT}. \quad (3-35)$$

For a small number of important moderator materials, the scattering law is tabulated in ENDF/B as piecewise continuous functions over a set of discrete α and β values with an interpolation law describing the variation between the tabulated points. In the RACER system, these are converted into cumulative distribution functions for a number of incident energies, exit energies, scattering angles, and temperatures. Typical values are 54 incident energies, 80 exit energies, 80 scattering angles, and six temperatures. Adjustment of the data to the actual moderator temperature is performed as described by Ballinger [1995]. For materials for which tabulated $S(\alpha, \beta)$ data are not available, a free-gas scattering law approximation is utilized.

Coherent Elastic Scattering

The double differential coherent elastic scattering cross section is represented as

$$\sigma_s(E \rightarrow E', \mu, T) = \frac{1}{E} \sum_{i=1}^{E_i < E} s_i(T) \delta(\mu - \mu_i) \delta(E - E'), \quad (3-36)$$

where T is the ambient temperature, s_i is a combined crystallographic structure and Debye-Waller factor, and E_i and μ_i are the associated Bragg edge energies and scattering cosines. In the MCV algorithm, scattering of a neutron with incident energy E from the j^{th} lattice plane is sampled with probability $s_j / \sum_{i=1}^{E_i < E} s_i$. The scattering cosine is then given by

$$\mu_j = 1 - \frac{2E_j}{E}. \quad (3-37)$$

The exit energy is the same as the incident energy.

Incoherent Elastic Scattering

The double differential scattering cross section for some partially ordered materials, such as ZrH_x and polyethylene, may be treated using the incoherent approximation,

$$\sigma_s(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2} e^{-2EW'(T)(1-\mu)} \delta(E - E'), \quad (3-38)$$

where σ_b is the characteristic bound cross section, $W'(T)$ is the Debye-Waller integral divided by the atomic mass, and T is the ambient temperature. These parameters are obtained from the ENDF/B files. The cumulative distribution function for the scattering cosine may be obtained from Eq. (3-38) as

$$P_{\text{incoherent elastic}}(\mu) = \frac{\int_{-1}^{\mu} \int \sigma_s(E \rightarrow E', \mu', T) dE' d\mu'}{\int_{-1}^{\mu} \int \sigma_s(E \rightarrow E', \mu', T) dE' d\mu'} = \frac{e^{2EW'\mu} - e^{-2EW'}}{e^{2EW'} - e^{-2EW'}}. \quad (3-39)$$

Inverting this expression, the scattering cosine is thus sampled using

$$\mu = \frac{\ln[\xi(e^{2EW'} - e^{-2EW'}) + e^{-2EW'}]}{2EW'}, \quad (3-40)$$

where ξ is a random number drawn on (0,1).

4. TALLIES AND EDITS

As the neutron histories are being followed, *tallies* are accumulated that are later used to compute the results requested by the user. These results are referred to as *edits*. In Section 4.1 the types of tallies are described. In Section 4.2 the various types of edits and how they are computed are discussed. For each type of edit there is also an explanation of how the uncertainty on the quantity is determined. Finally, Section 4.3 gives a very brief discussion of the source normalization correction that is optionally applied to the results of iterated-source calculations.

4.1 TALLIES

When the regular tracking scheme is invoked MCV uses two estimators: the path-length estimator and the collision estimator [Carter and Cashwell, 1975]. Path-length estimators are tallied during the neutron tracking operations, while collision estimators are tallied during the collision analysis operations. The estimators are accumulated for each edit group and edit medium. The relative performance of two estimators (in terms of the variance) depends on the physical problem [MacMillan, 1966]. The path-length estimator tends to perform better for optically-thin regions, while the collision estimator can perform better for optically-thick regions. MCV normally combines the results of the two estimators to obtain an optimal edited value, as described in Section 4.2.

4.1.1 The Path-Length Estimator

A *track* is defined as the path followed by a neutron from one boundary crossing to another, from one collision to another, from a boundary crossing to a collision, or from a collision to a boundary crossing. Denote the path-length estimator for a reaction rate of type x ($x = \{a, f, n\}$ for absorption, fission, or ν -fission, respectively), in edit group G , by $R_{p,x}^G$. When a neutron with an energy lying in subgroup i in edit group G in the fast range creates a track of length t in edit medium n , the path-length estimator for reaction type x is updated using the replacement operation

$$R_{p,x}^G \leftarrow R_{p,x}^G + wt \frac{v_i}{v} \Sigma_{x,i,m_n}, \quad (4-1)$$

where w is the history weight, v is the neutron speed, v_i is the speed at the midpoint of the subgroup, and Σ_{x,i,m_n} is the macroscopic cross section at the midpoint of the subgroup for reaction type x in material m_n that comprises edit medium n . In the thermal group, the replacement operation is given by

$$R_{p,x}^G \leftarrow R_{p,x}^G + wt \Sigma_{g,m_n}, \quad (4-2)$$

where g denotes the thermal group.

4.1.2 The Collision Estimator

Denote the collision estimator for a reaction rate of type x , in edit group G by $R_{c,x}^G$. When a neutron with an energy lying in subgroup i in edit group G in the fast range undergoes a collision in edit medium n , the collision estimator for reaction type x is updated using the replacement operation

$$R_{c,x}^G \leftarrow R_{c,x}^G + w \frac{\Sigma_{x,i,m_n}}{\Sigma_{t,i,m_n}} \quad (4-3)$$

In the thermal range, the equivalent expression is

$$R_{c,x}^G \leftarrow R_{c,x}^G + w \frac{\Sigma_{x,g,m_n}}{\Sigma_{t,g,m_n}} \quad (4-4)$$

4.1.3 Tallies During Delta Tracking

Path-length tallies are not possible when using delta-tracking since track lengths are not available on a region-wise basis. Collision tallies may be performed, however, for all pseudocollisions. The procedure is the same as for the case of no delta-tracking, except that the total cross section appearing in equations (4-3) and (4-4) is replaced by the reciprocal of the minimum mfp used for the delta-tracking.

4.1.4 Additional Tallies and Options

Energy loss due to elastic and inelastic scattering are separately obtained by tallying $w'(E' - E)$ at each collision, where E and E' are the pre- and post-collision energies, respectively, and w' is the post-collision weight. Leakage and slowing-down are tallied using analog estimators. Finally, the user may optionally cause the nuclidic reaction rate estimator to be the arithmetic mean of the path-length and collision estimators. This reduces the storage required for these quantities by a factor of two since one variable is used to accumulate both estimators.

4.2 EDITS

Edits refer to the results generated by MCV. These quantities may be formatted for direct inspection by the user or they may be binary values written to a file for use by another code. During the tracking operations, edit-medium-and-edit-group-integrated reaction rates and fluxes are tallied on a batch-wise basis. Following the tracking, the batch-wise values are combined to yield the edited results. In addition to the edit-medium integrated reaction rates and fluxes, MCV can also compute *combination edits* (sums of other edits) and *ratio edits* (ratios of other edits). Section 4.2.1 discusses the computation of the edits and their uncertainties when just one estimator is used, and Section 4.2.2 describes how these quantities are obtained when both path-length and collision estimates are available. Section 4.2.3 discusses the special case of ratio edits.

4.2.1 Single Estimator

In some cases, such as when delta-tracking is being used, MCV computes a single estimate of a given quantity for each of N non-discarded batches. These batch-wise values are used to provide both an estimate of the quantity as well as an indication of the uncertainty on the estimate.

Mean Value

The primary edited result is given simply as the arithmetic mean, m_1 , of the batch-wise values, i.e.,

$$m_1 = \frac{1}{N} \sum_{i=1}^N x_i, \quad (4.5)$$

where x_i is the estimator value for batch i and the sum is over the non-discarded batches.

95 Percent Confidence Interval

Assuming that the batch-wise values are statistically-independent, an estimate of the standard deviation of the mean value may be determined as

$$s = \sqrt{\frac{m_2}{N-1}}, \quad (4.6)$$

where

$$m_2 = \frac{1}{N} \sum_{i=1}^N (x_i - m_1)^2. \quad (4.7)$$

For iterated-source calculations the assumption of statistical independence is not strictly valid [MacMillan, 1973]. For these calculations the alternative expression

$$s = \max \left[\sqrt{\frac{m_2}{N-1} \left(1 + \frac{2r}{1-\delta} \right)}, \sqrt{\frac{m_2}{N-1}} \right] \quad (4.8)$$

may be used, where r is an estimate of the correlation coefficient and δ is the dominance ratio (i.e., the ratio of the first harmonic and fundamental mode eigenvalues). The correlation coefficient is estimated as

$$r = \frac{(N-1) \sum_{i=1}^{N-1} x_i x_{i+1} - \sum_{i=1}^{N-1} x_i \sum_{j=2}^N x_j}{\sqrt{\left[(N-1) \sum_{i=1}^{N-1} x_i^2 - \left(\sum_{i=1}^{N-1} x_i \right)^2 \right] \left[(N-1) \sum_{i=2}^N x_i^2 - \left(\sum_{i=2}^N x_i \right)^2 \right]}}, \quad (4.9)$$

and the dominance ratio is supplied by the user. The use of Eq. (4-8) approximately corrects for correlation effects when the estimate of the correlation coefficient is positive but not when the coefficient is negative, thus always providing a conservative estimate of the standard deviation.

Assuming that the batch-wise values are drawn from a normal distribution, the 95 percent confidence interval to contain the true mean is $(m_1 - t_{N-1}(0.975)s, m_1 + t_{N-1}(0.975)s)$, where $t_{N-1}(0.975)$ is the 95 percent t statistic for $N-1$ degrees of freedom. To indicate the degree of uncertainty of the edited mean values, MCV also normally edits the half-width of this interval, i.e., $d = t_{N-1}(0.975)s$.

Since the half-width estimate given is only valid if the batch-wise estimates are drawn from a normal distribution, MCV performs a normality test. First, the skewness coefficient is estimated as

$$\hat{\gamma} = \sqrt{\frac{N-1}{N}} \frac{m_3}{m_2^{3/2}}, \quad (4-10)$$

where

$$m_3 = \frac{1}{N} \sum_{i=1}^N x_i^3 - 3m_1m_2 - m_1^3. \quad (4-11)$$

For the special case of $m_2 = 0$ Eq. (4-11) is not used, and the skewness coefficient is set to zero. Then, if

$$\hat{\gamma}^2 \geq t_{\infty}^2(0.975) \left[\frac{6(N-1)(N-2)}{N(N+1)(N+3)} \right] \max \left[1, 1 + \frac{2r^3}{1-\delta^3} \right], \quad (4-12)$$

the confidence interval is flagged with a symbol in the output to indicate that it is of doubtful validity. If

$$\hat{\gamma}^2 \geq t_{\infty}^2(0.9975) \left[\frac{6(N-1)(N-2)}{N(N+1)(N+3)} \right] \max \left[1, 1 + \frac{2r^3}{1-\delta^3} \right], \quad (4-13)$$

then the confidence interval is flagged with a symbol to indicate that it is probably meaningless. If confidence intervals are not being corrected for source correlation, then $r = 0$ in Eqs. (4-12) and (4-13).

4.2.2 Double Estimators

In the most general case, MCV computes both a path-length and a collision estimate for a given quantity for each non-discarded batch. The batch-wise values of both types of estimators are combined to yield optimal estimates of the mean values and their uncertainties.

Mean Value

Denoting the path-length and collision estimates of an edited quantity for non-discarded batch i as $x_{p,i}$ and $x_{c,i}$, respectively, the mean values m_p and m_c are determined for each using Eq. (4-5). Second moments about the mean values, m_{pp} and m_{cc} , are also computed using Eq. (4-7), as is the cross covariance

$$m_{pc} = \frac{1}{N} \sum_{i=1}^N x_{p,i}x_{c,i} - m_p m_c. \quad (4-14)$$

and the quantity

$$\alpha = \frac{m_{cc} - m_{pc}}{m_{cc} - 2m_{pc} + m_{pp}} \quad (4-15)$$

The edited mean value m_1 is then determined according to the following prescription:

- if $m_c = 0$ then $m_1 = m_p$; else
- if $\alpha > 1$ then $m_1 = m_p$; else
- if $\alpha < 0$ then $m_1 = m_c$;
- otherwise,

$$m_1 = \alpha m_p + (1 - \alpha) m_c \quad (4-16)$$

The logic behind this scheme is that Eq. (4-16) is the linear combination of the two estimators that has the minimum variance. This expression is only used in the range $0 < \alpha < 1$ so that the edited value lies between the value of the two estimators. If α falls outside this range, then the appropriate single estimator is used. If, however, the collision estimate is identically zero, then just the path-length estimate is used. This is to avoid the situation that can arise when neutrons stream through an edit medium without colliding. In this case, the path-length estimator can be non-zero with a non-zero variance, but the collision estimator will be zero with a zero variance. The coefficient α will then evaluate to zero, and the edited result would be solely due to the undersampled collision estimator.

95 Percent Confidence Interval

The 95 percent confidence interval calculations are the same as for the case of a single estimator, except that

$$m_2 = \alpha^2 m_{pp} + 2\alpha(1 - \alpha) m_{pc} + (1 - \alpha)^2 m_{cc} \quad (4-17)$$

and

$$r = \alpha r_p + (1 - \alpha) r_c, \quad (4-18)$$

where r_p and r_c are given by Eq. (4-9) but with x_i replaced by $x_{p,i}$ and $x_{c,i}$, respectively. The normality test uses Eqs. (4-10), (4-12), and (4-13) as in the case for a single estimator. The value of m_3 , however, is given by

$$m_3 = \frac{1}{N} \left[\alpha^3 \sum_{i=1}^N x_{p,i}^3 + 3\alpha(1 - \alpha) \left(\alpha \sum_{i=1}^N x_{p,i}^2 x_{c,i} + (1 - \alpha) \sum_{i=1}^N x_{p,i} x_{c,i}^2 \right) + (1 - \alpha)^3 \sum_{i=1}^N x_{c,i}^3 \right] - 3m_1 m_2 - m_1^3 \quad (4-19)$$

4.2.3 Ratio Edits

Ratio edits are simply the ratio of two other edited quantities. Ratio edits normally use only the path-length estimator. (The exception is the case where a single estimator that is the arithmetic average of the path-length and collision estimators is used.)

Mean Value

Let x_i and y_i be the estimator values for the numerator and denominator, respectively, for batch i . The mean values of the batch-wise estimates, m_x and m_y , are determined using Eq. (4-5). The edited ratio is given by

$$m_1 = m_x/m_y. \quad (4-20)$$

95 Percent Confidence Interval

The 95 percent confidence interval calculation is the same as described in Section 4.2.1, with the following redefinitions:

$$m_2 = \left[\frac{m_x}{m_y} \right]^2 \left[\frac{m_{xx}}{m_x^2} - 2 \frac{m_{xy}}{m_x m_y} + \frac{m_{yy}}{m_y^2} \right] \quad (4-21)$$

and

$$r = \frac{\frac{\sum_{i=1}^{N-1} x_i x_{i+1}}{m_x^2} - \frac{\sum_{i=1}^{N-1} (x_{i+1} y_i + x_i y_{i+1})}{m_x m_y} + \frac{\sum_{i=1}^{N-1} y_i y_{i+1}}{m_y^2}}{\left[\frac{\sum_{i=1}^{N-1} x_i^2}{m_x^2} - 2 \frac{\sum_{i=1}^{N-1} x_i y_i}{m_x m_y} + \frac{\sum_{i=1}^{N-1} y_i^2}{m_y^2} \right] \left[\frac{\sum_{i=2}^N x_i^2}{m_x^2} - 2 \frac{\sum_{i=2}^N x_i y_i}{m_x m_y} + \frac{\sum_{i=2}^N y_i^2}{m_y^2} \right]}, \quad (4-22)$$

where

$$m_{xx} = \frac{1}{N} \sum_{i=1}^N (x_i - m_x)^2,$$

$$m_{yy} = \frac{1}{N} \sum_{i=1}^N (y_i - m_y)^2,$$

and

$$m_{xy} = \frac{1}{N} \sum_{i=1}^N x_i y_i - m_x m_y.$$

Normality testing is not performed for ratio edits.

4.3 SOURCE NORMALIZATION CORRECTION

The use of a fixed number of histories per batch in iterated source calculations leads to a bias in the results [Lieberoth, 1968]. MCV optionally employs an approximate scheme to correct for this bias. Let K_i be the ratio of the neutron production to neutron source for batch i , and let

$$K = \left(\prod_{i=1}^N K_i \right)^{1/N} \quad (4-23)$$

be the geometric mean over all non-discarded batches. A source normalization weight of $M_1 = 1$ is assigned to the first batch, and weights for subsequent batches are determined using

$$M_i = \frac{K_{i-1}}{K} M_{i-1}. \quad (4-24)$$

For the case of a single estimator, the weighted average

$$\bar{x} = \frac{\sum_{i=1}^N M_i x_i}{\sum_{i=1}^N M_i} \quad (4-25)$$

is given as the edited quantity rather than the value of m_1 . For the case of double estimators, weighted averages \bar{x}_p and \bar{x}_c are computed for the path-length and collision estimates in the same manner. These are then combined to yield the edited result based on the value of α as described in Section 4.2.2. Similarly, ratio edits are the ratio of weighted averages for the numerator and denominator. The calculation of confidence intervals is unaffected by the source normalization correction procedure.

5. STRATEGIES FOR RUNNING THE CODE

5.1 SOURCE GUESS AND CONVERGENCE FOR ITERATED-SOURCE CALCULATIONS

In the absence of *a priori* knowledge of the converged source shape, a good choice for the initial source distribution is one that is uniform over all fuel-bearing regions. To implement this in a calculation, the user specifies that initial source sites may only be located within certain edit media within a certain user-defined box as described in Section 3.2.1. It is up to the user to ensure that all fuel-bearing regions are included in the list of valid edit media as well as within the box. Another possibility is a uniform distribution over some volume that contains every fuel-bearing region. To implement this in a calculation, the user simply specifies a box known to enclose all fuel-bearing regions. No specific edit media are specified, and thus neutrons can start anywhere within the box. The first option generally takes longer in the initial source generation phase since sites initially placed in non-fuel-bearing regions within the box are rejected, but results in a more realistic initial source distribution which can reduce the number of batches that must be discarded. In either case, it is important that every fuel-bearing region be included in the initial source volume, as this is more likely to cause the source to converge quicker and also to reduce the potential of undersampling some regions during the initial portion of the calculation. The use of a converged source distribution—for example from the previous depletion time step—can cause the source to converge much faster.

Since the initial source distribution will in general not be that of the converged distribution, tallies obtained prior to the source being sufficiently converged should not be included in the results. This is accomplished by specifying a number of batches to discard. Tallies are not scored or accumulated for discarded batches. Plots of selected batch-averaged results versus the initial number of batches discarded are a good way to determine how many batches to discard for a particular application. In general, the asymptotic convergence rate will depend on attributes of the physical model such as core size, neutron mean-free-path, neutron lifetime, etc.

For highly decoupled configurations, one should watch for step changes in batch-wise results. This can indicate that some region of the model was undersampled in the batches prior to the step change.

5.2 NUMBER OF HISTORIES AND BATCHES

For fixed-source calculations the accuracy of the results depends only on the net number of histories run, and not on how they were partitioned into batches. The statistical analysis of the uncertainty, however, is more accurate if the histories are divided into more batches. Code performance, however, favors larger batches and some trade-off must be found. The situation is more complicated for iterated-source calculations due to the need to discard initial batches and the bias that increases as the number of histories per batch decreases. Common practice is to utilize batch sizes of tens to hundreds of thousands of histories, to discard several tens of batches for iterated source calculations, and to accumulate tallies for a few hundred batches.

5.3 VARIANCE REDUCTION

Variance reduction schemes used in MCV include rouletting, splitting, and delta-tracking. It can be shown that a statistically-optimum Monte Carlo calculation is one in which the weight of each neutron upon exiting a collision or crossing a boundary is inversely proportional to the expected subsequent score for the estimator for which the calculation is being optimized. Weight standards, therefore, should be chosen to cause this to happen as nearly as possible. For iterated-source calculations performed for core physics analyses, it has been found through experience that set-

ting the minimum and nominal weight standards to one-half the maximum standard, and the standards in the reflector to twice the values in the core, yields adequate performance.

The optimal use of delta-tracking is dependent on both the physical problem, the characteristics of the computer used, and computational environment in which the calculation is performed. For light water reactors good performance has been obtained using delta-tracking only for energies above approximately 10 eV.

5.4 PHYSICS TREATMENT OPTIONS

The following are the recommended physics treatments:

- use the free gas model for scattering from bound hydrogen for all energies in the fast range,
- use the isotropic-in-the-center-of-mass option versus the isotropic-in-the-laboratory option for inelastic scattering, and
- use the continuous-energy thermal range treatment versus the multigroup treatment.

5.5 COMPUTER-DEPENDENT OPTIONS

MCV uses a master/slave model to support message-passing, distributed-memory computing. There is one master instance of the code that coordinates the work of and receives tallies from one or more slave instances. Each slave is multitasked using a shared-memory-parallelism (SMP) model. The memory required for the slaves is proportional to the number of instances of the slaves. The memory requirement is independent of the number of processors assigned to the slaves for SMP multitasking. Often a good strategy is to use SMP parallelism to the maximum extent that the hardware will permit, i.e., up to the number of processors sharing memory in one 'box'; and to use message-passing between boxes. Inefficiencies in the management of memory conflicts as multiple processors access shared memory may lead to message-passing within a box at the cost of greater memory requirements.

For a fixed number of histories per batch the addition of processors will at first result in the completion of the calculation in less wall-clock time, but eventually a point will be reached beyond which additional processors will slow the calculation. For a given application one must determine the optimal number of processors to use by trial-and-error. Alternatively, performance may be improved by increasing the number of histories per batch.

6. INPUT OPTIONS

In this section, all of the available input options to the MCV module are summarized. The options are correct for version MCV.14.3. In what follows, the name 'Datatran' [Kopp, 1977] refers to an input-processing language. The following general rules apply:

- All entries occur in pairs, where the first item is a "keyword" identifying an option, and the second item is the user-selected "value" for the option.
- All "keyword, value" pairs are optional, with defaults provided if the pair is not present. The default values are indicated below either by underlining the default value (e.g., value) or by placing the default value in brackets (e.g., {value}).
- The "keyword, value" pairs may be specified in any order. If a particular "keyword, value" pair is specified more than once, only the last occurrence is used.
- For initial jobs any of the entries may be supplied.
- For restart calculations to run more neutron histories, only the "BATCHES, n" and "NPROCMCV, n" entries may be changed - all other entries are ignored.
- In the description below, user-supplied values are denoted by "n" for integer quantities, "x" for real (floating-point) quantities, and "c" for character or Hollerith quantities. Normal Datatran conventions are adhered to (i.e., numbers may be input either as integers or reals, Hollerith data may be entered directly if it begins with a letter or enclosed in asterisks, the F.ZZZ form may be used to supply Fortran variables, the N.ZZZ form to supply other Datatran lists, etc.).
- Datatran lists followed by *[external]* refer to lists specified via the input processors.

The input options are grouped into categories as follows:

- General input and options
- Physics options
- Edits and output options
- Siteplot and fission-matrix options
- Detector response kernels
- Variance reduction options
- Alpha-mode calculations
- Perturbation theory

6.1 GENERAL INPUT AND OPTIONS

The following pairs of "keyword, entry" provide general options pertaining to the running strategy and overall control of the calculation:

NPROCMCV, <i>n</i>	{1} Number of slave processes (pvm processes). Must be less than 32. May be changed for restart calculations.
BATCHES, <i>n</i>	{25} Number of batches. RACER will terminate after fewer batches, if necessary, in order to provide for file wrap-up before time limits are reached. For a depletion job, this entry applies to each timestep. May be changed for restarts.
NEUTRONS, <i>n</i>	{16000} Number of histories per batch. Recommended: 10-20 K histories for each slave

macrotask, e.g., NPROCMCV·NCPUS·10,000. (NCPUS is a UNIX environment variable used to specify the number of processors assigned to each macrotask.)

DISCARD, <i>n</i>	{0} Number of initial batches to discard. "Discarded" batches are not edited. The N.BATCHED input for RACED should specify that batches starting with (<i>n</i> +1) should be edited. RACER will check the N.BATCHED list and override the "DISCARD, <i>n</i> " input if necessary such that no discarded batches will be edited.
SORSOPT, <i>c</i>	Source option.
<u>ITERATE</u>	Iterated-fission problem. For batch 1, the source shape is taken from the RACER010 file; otherwise generated internally based on the N.SOURCE [<i>external</i>] input parameters.
FIXED	Fixed-source for all batches, based on the N.SOURCE [<i>external</i>] input parameters.
FIXITER	Special iterated-fission problem, where the source spectrum for batch 1 is that specified via N.SOURCE [<i>external</i>] input and the source spectrum for all subsequent batches is the standard prompt plus delayed fission spectrum.
MULTFIX	Multiplied fixed source calculation.
JOBTYPE, <i>c</i>	Control for batch-wise output.
<u>NORMAL</u>	The initial batch number for the calculation is determined by adding 1 to the last batch number obtained from the RACER010 file. If RACER010 is not present, then the initial batch is designated as "batch 1." Other quantities (e.g., FISWTLOW, cumulative eigenvalue, etc.) are also obtained from RACER010 if present. This option is intended for all BOL jobs (both initial jobs and restarts).
DEplete	The initial batch number for the calculation is reset & designated as "batch 1." The source from RACER010 is used if available, but other quantities (e.g., FISWTLOW, cumulative eigenvalue, etc.) are ignored & reset. This option is intended for depletion calculations. The JOBTYPE,DEplete option may also be used for non-depleting problems where an initial source guess (RACER010) from a different problem is to be used. Such a source guess is appropriate only if the geometry for the previous problem is identical in all respects to that for the new problem.
FISWTLOW, <i>x</i>	{.8} Average weight for selecting fission sites in iterated-fission problems. Used for the initial batch, and should be slightly less than the estimated problem eigenvalue. In general, the default value is suitable for all problems.
VRNSEED, <i>n</i>	{93409695577021} Any odd integer ($< 2^{48}-1$) to be used as the random number seed (for initial jobs only).
NDELTA, <i>n</i>	Number of edit-groups in which delta-tracking is to be used. The maximum number of edit-groups for which delta-tracking may be selected is 9.
DELTA _{<i>j</i>} , <i>n_j</i>	Use delta tracking in edit-group <i>n_j</i> . Up to 9 entries may be input, but only the first NDELTA entries will be used.
MAXVLDYN, <i>n</i>	{2048} Maximum length used for scratch vectors in MCV. In general, do not use this option.
CLUSTERS, <i>n</i>	Strategy for scratch file usage, for job-specific supergroup cross-section scratch files.
<u>-1</u>	Create & use racerxs* scratch files.
0	Keep all scratch cross-sections in shared memory, no disk storage.

6.2 PHYSICS OPTIONS

PTURR, <i>c</i>	Probability table method for unresolved resonances (fast neutron physics).
<u>NO</u>	Use the standard dilute-average cross-sections
YES	Use the PTURR data files as specified in RACER_PTURR
DOPPLER, <i>c</i>	In-RACER Doppler broadening to the material temperature specified in the input.
<u>NO</u>	Do not Doppler broaden. Use existing EVDF library data.
YES	Doppler broaden the supplied cross-sections.
SABOPT, <i>c</i>	Continuous-energy physics option for the thermal range.
<u>YES</u>	Use continuous-energy thermal neutron treatment.
NO	Use multigroup treatment.
NSUBSAB, <i>n</i>	{1000} Number of energy subgroups contained within the thermal supergroup when the continuous-energy treatment is used. Ignored if the N.ESUBSAB [external] list is used.
FGECUT, <i>x</i>	{10 ⁷ } Upper energy limit (in eV) for use of the free-gas model for bound-hydrogen scatter.
RDS6, <i>c</i>	Upper energy value for the MUFT energy group structure.
<u>NO</u>	Use 20 MeV for the top energy of MUFT group 1 and treat multigroup background fission product data as group-averaged.
YES	Use 10 MeV for the top energy of MUFT group 1 and treat multigroup background fission product data as pointwise.
ZEROXSEC, <i>c</i>	{NONE} Zero-out the microscopic cross-sections for one nuclide. (Actually, multiply by 10 ⁻²⁰ .) "c" should be the nuclide alias which appears on the N.ISOT [external] list. (If an alias is not specified, supply the nuclide name.) Only one name may be specified.
FIXNEGXS, <i>c</i>	Control of negative microscopic cross-sections.
<u>NO</u>	Negative microscopic cross-sections are permitted.
YES	Set negative microscopic cross-sections to zero.
FIXINEL, <i>c</i>	Control of warning messages for inconsistent inelastic scattering matrix elements.
<u>NO</u>	Do not alter the weight multipliers associated with the inelastic scattering energy transfer.
YES	Replace all weight multipliers of 0.0 by 10 ⁻²⁰ , for the weight multipliers associated with the inelastic scattering energy transfer. This eliminates warning messages for some minor inconsistencies between the inelastic microscopic cross-section & the associated energy transfer matrix.
HEAYVBND, <i>c</i>	Chemical binding correction to fast-range scattering for heavy nuclides (A>1.25).
<u>NO</u>	Do not apply the heavy-nuclide binding model.
YES	Use the "effective alpha" model. (Must also supply "HEAYVTEV, x".)
HEAVYTEV, <i>x</i>	{0.0} The effective temperature in electron-volts to be used in the effective-alpha model for heavy-nuclide scattering binding corrections. If "x" is negative, the same effective temperature as for the bound-hydrogen binding correction will be used. This entry must be supplied if "HEAYVBND, YES" is selected.
INELMASS, <i>n</i>	Option for inelastic scattering.
<u>0</u>	Treat inelastic scattering as isotropic in the laboratory system.
1	Treat inelastic scattering as isotropic in the center-of-mass system.

INTERPTH, <i>n</i>	Option for temperature interpolation of thermal multigroup cross-section data.
0	Use T_F^2 (T_F is temperature in degrees Fahrenheit).
1	Use $\sqrt{T_R}$ (T_R is temperature in degrees Rankine).
NSTEPS, <i>n</i>	{31} Number of equiprobable cosine-bins to use for fast-range angular distributions.
CNDFELIB, <i>n</i>	{5} Specifies the integer value associated with the "ng" parameter of CNDF file names having endings of "ng, nf, nt". The CNDF file names have endings of "5, 1, 1" for the standard 32-multigroup libraries using a breakpoint of 0.625 eV. The only permitted values of <i>nf</i> and <i>nt</i> are still "1, 1".

6.3 EDITS AND OUTPUT OPTIONS

PTURRED, <i>c</i>	Provide detailed and voluminous edits of the entire set of PTURR data for the problem.
NO	Save a tree.
YES	Provide the edits.
SUM24NEW, <i>c</i>	Use the new unblocked file format for the RACERSUM and RACER024 files.
NO	Standard format.
YES	New, unblocked format - more efficient for very large jobs.
RACED, <i>c</i>	Control for in-line editing of results with statistics.
NO	Produce the RACER002 scratch file of batch results, and use the stand-alone RACED module for editing. Must also specify "N.RACER = RACER RACED".
YES	Perform in-line editing of batch results, and do not produce the RACER002 file. M-factors cannot be used when this option is selected. Must also specify "N.RACER = RACER".
OPTAGE, <i>c</i>	Control for edits of the neutron slowing down age, in units of cm^2 .
NO	Do not tally and edit the neutron age.
YES	Tally and edit the neutron age.
OPTLIFE, <i>c</i>	Control for edits of the average neutron lifetime, in units of seconds.
NO	Do not tally and edit the neutron lifetime.
YES	Tally and edit the neutron lifetime.
OPTLEAK, <i>c</i>	Edit the net leakage for each edit-medium, labelled as "LEAKAGE (NET)".
NO	Do not edit net leakage for edit-media.
YES	Edit net leakage.
OPTLOSS, <i>c</i>	Select the "energy loss" edit option. Produce additional edits for each edit-medium of the energy loss in eV due to neutron elastic scattering (labelled "ELASTIC-ENERGY-LOSS") & the energy loss in eV due to neutron inelastic scattering (labelled "INELAST-ENERGY-LOSS").
NO	Do not generate energy loss edits.
YES	Produce the energy loss edits.
SURFEDIT, <i>c</i>	Control for the surface-edits, where special nuclidic edits are created for entering and leaving each bounding surface of each sector in the problem.
NO	Do not produce surface-edits.

YES	Produce surface-edits of the number, flux, and current.	
NUMBER	Produce surface-edits only for the number of crossings (not for flux and current).	
MEDTRKED, <i>c</i>	Controls the option of tallying the number of flights and collisions occurring in each edit medium.	
NO	Do not tally flights and collisions for edit medium.	
YES	Tally flights and collisions for edit medium	
EDITS, <i>c</i>	Controls the printing of output from RACED or in-line RACED routines.	
YES	All edits are printed to paper. The RACEROUT and RACERSUM files are written.	
NO	No edits are printed to paper, however the RACEROUT file is still written.	
PART	All edits except nuclidic edit descriptions and nuclidic edits are printed to paper. The RACEROUT and RACERSUM files are written which contain nuclidic edits.	
REEDIT, <i>c</i>	Specifies whether or not the job is a re-edit job. If the job is a re-edit job, RACED will use the RACERIN and RACER024 files to print all edits to paper output. This option is only meaningful for the stand-alone RACED, and cannot be used with in-line editing.	
NO	Normal RACED execution.	
YES	Edit the information contained on RACERIN to paper.	
BATCHCOR, <i>c</i>	Specifies whether or not to apply the source correlation correction factor to confidence intervals.	
YES	Apply source correlation correction.	
NO	Do not apply source correlation correction.	
DOMRATIO, <i>x</i>	{0.9} Dominance ratio to use in the correction of confidence intervals for source correlation.	
MFACTORS, <i>c</i>	Specifies whether or not to apply the source normalization weights or M-factors to account for the relative weights in each batch in an iterated source problem. This option can be used only with stand-alone RACED, and is ignored with in-line editing.	
YES	Apply M-factors (if stand-alone RACED).	
NO	Do not apply M-factors. This option will be chosen automatically if the BIGDEPL or "RACED, YES" options are in use.	
IPRTGRD, <i>n</i>	Edit control for grid summary edits from RACER3D,	0=no, 1=yes.
IPRTSECT, <i>n</i>	Edit control for sector summary edits from RACER3D,	0=no, 1=yes.
IPRTSURF, <i>n</i>	Edit control for surface summary edits from RACER3D	0=no, 1=yes.
IPRTMATI, <i>n</i>	Edit control for material/edit/permutation summary edits,	0=no, 1=yes.
IPRTMIC, <i>n</i>	Edit control for generating data files for all pointwise xsec data,	0=no, 1=yes.
IPRTINEL, <i>n</i>	Edit control for printing inel-matrix alias sampling setup,	0=no, 1=yes.
IPRTIMPR, <i>n</i>	Edit control for printing importance weights,	0=no, 1=yes.
IPRTISED, <i>n</i>	Edit control for printing nuclidic edit definitions,	0=no, 1=yes.
IPRT24, <i>n</i>	Debug print for all of RACER024 file,	0=no, 1=yes.
IPRTMAT, <i>n</i>	Edit control for printing material composition specs,	0=yes, 1=yes, -1=no.

6.4 SITEPLOT AND FISSION MATRIX OPTIONS

FMATRIX, <i>c</i>	Controls the generation of a fission matrix and corresponding eigenvalue and eigenvector by MCV. As long as "ACCELER, NO" (the default) is selected, this option will not affect results or random number sequences. The additional keyword/value pairs which define the site-grid are required if this option is selected (SITEINTX, SITEINTY, SITEINTZ, SITEXMIN, SITEXMAX, SITEYMIN, SITEYMAX, SITEZMIN, SITEZMAX).
<u>NO</u>	Do not generate the fission matrix.
YES	Generate the fission matrix, its eigenvalue, and its eigenvector.
ADJOINT	Generate the adjoint fission matrix.
SITEPLOT, <i>c</i>	Controls the generation of data for graphics display of source convergence. If selected, the source sites at the beginning of each batch are tallied on the fission matrix grid and included in the RACER011 file for post-processing. The additional keyword/value pairs which define the site-grid are required if this option is selected (SITEINTX, SITEINTY, SITEINTZ, SITEXMIN, SITEXMAX, SITEYMIN, SITEYMAX, SITEZMIN, SITEZMAX).
<u>NO</u>	Do not generate data for batch-wise source graphics.
YES	Generate data for batch-wise source convergence monitoring and include the data in the RACER011 output file.
BATCH	Same as "YES".
CUM	Generate data for the source convergence monitoring at job completion (cumulative) and include the data in the RACER011 output file.
SITEUNIT, <i>c</i>	Specifies the units for the SITEXMIN, SITEXMAX, SITEYMIN, SITEYMAX, SITEZMIN, SITEZMAX entries below.
<u>CM</u>	Units of centimeters for the site grid boundaries
IN	Units of inches for the site grid boundaries
SITEINTX, <i>n</i>	{10} Number of intervals in the x-direction for the site grid.
SITEINTY, <i>n</i>	{10} Number of intervals in the y-direction for the site grid.
SITEINTZ, <i>n</i>	{1} Number of intervals in the z-direction for the site grid.
SITEXMIN, <i>x</i>	{-1000.} Value of x at the minimum-x boundary of the site grid.
SITEXMAX, <i>x</i>	{1000.} Value of x at the maximum-x boundary of the site grid.
SITEYMIN, <i>x</i>	{-1000.} Value of y at the minimum-y boundary of the site grid.
SITEYMAX, <i>x</i>	{1000.} Value of y at the maximum-y boundary of the site grid.
SITEZMIN, <i>x</i>	{-1000.} Value of z at the minimum-z boundary of the site grid.
SITEZMAX, <i>x</i>	{1000.} Value of z at the maximum-z boundary of the site grid.
FEIGPLOT, <i>c</i>	Controls the generation of data for graphics display of fission matrix eigenvector convergence. If selected, fission matrix eigenvector for each batch is included in the RACER011 file for post-processing. The additional keyword/value pairs which select the fission matrix option and define the site-grid are required if this option is selected (FMATRIX, SITEINTX, SITEINTY, SITEINTZ, SITEXMIN, SITEXMAX, SITEYMIN, SITEYMAX, SITEZMIN, SITEZMAX).

<u>NO</u>	Do not output the fission matrix eigenvector graphics data.
YES	Generate data for batch-wise monitoring of the fission matrix eigenvector and include the data in the RACER011 output file.
BATCH	Same as "YES".
CUM	Generate data for the fission matrix eigenvector at job completion (cumulative) and include the data in the RACER011 output file.
FMATPLOT, <i>c</i>	Controls the generation of data for graphics display of fission matrix convergence. If selected, the entire (cumulative) fission matrix after each batch is included in the RACER011 file for post-processing. The additional keyword/value pairs which select the fission matrix option and define the site-grid are required if this option is selected (FMATRIX, SITEINTX, SITEINTY, SITEINTZ, SITEXMIN, SITEXMAX, SITEYMIN, SITEYMAX, SITEZMIN, SITEZMAX).
<u>NO</u>	Do not output the fission matrix graphics data.
YES	Generate data for batch-wise monitoring of the fission matrix and include the data in the RACER011 output file.
BATCH	Same as "YES".
CUM	Generate data for the fission matrix at job completion (cumulative) and include the data in the RACER011 output file.
ACCELER, <i>c</i>	Controls the use of the fission matrix to accelerate convergence of the source distribution. The additional keyword/value pairs which select the fission matrix option and define the site-grid are required if this option is selected (FMATRIX, SITEINTX, SITEINTY, SITEINTZ, SITEXMIN, SITEXMAX, SITEYMIN, SITEYMAX, SITEZMIN, SITEZMAX).
<u>NO</u>	Do not use the fission matrix to bias the source distribution
YES	Bias the source site sampling for discarded batches only, without adjusting weights. Non-discarded batches are sampled in the normal manner.
FAIR	Bias the source site sampling for discarded batches, without adjusting weights. Non-discarded batches also use biased sampling, but are weighted for a fair game.
FOREVER	Bias the source site sampling for all batches, without adjusting weights.

6.5 VARIANCE REDUCTION OPTIONS

SPLIT, <i>c</i>	Controls the splitting option in RACER.
<u>NO</u>	Do not split particles in RACER.
YES	Split particles in RACER according to user input. Use "old" procedure for random number seeds.
NEW	Split particles in RACER according to user input. Use "new" procedure for fully reproducible random number seeds.
Note: If NCPUS>1, then "split yes" is overridden & replaced by "split new".	
MAXSTACK, <i>n</i>	{0} Specifies the maximum neutron stack size in RACER. For non-splitting problems this value is set equal to the batch size. For problems where splitting is enabled, this value may have to be determined by trial and error to accommodate the additional particles created by splitting.
MXSPLN, <i>n</i>	{0} Maximum splitting factor. If $n > 0$, particles will not be split more than n -for-1.
MXRUSN, <i>n</i>	{0} Minimum kill parameter for rouletting. If $n > 0$, the probability of a Russian roulette kill will be no less than 1 -in- n .

6.6 ALPHA-MODE CALCULATIONS

ALPHAEIG, <i>c</i>	Select the alpha-mode eigenvalue calculation.
<u>NO</u>	Perform standard <i>k</i> -mode eigenvalue calculation.
YES	Perform alpha-mode calculation. Vary alpha until $k_{\text{eff}} = \text{SRCHKEFF}$.
ALPHAIN, <i>x</i>	{0.0} Initial guess for alpha, used when "ALPHAEIG, YES".
SRCHKEFF, <i>x</i>	{1.0} Target k_{eff} for alpha search, used when "ALPHAEIG, YES".

6.7 PERTURBATION THEORY

PERTURB, <i>c</i>	Controls the perturbation of material densities.
<u>NO</u>	Ignore N.PERTURB, do not perform density perturbation calculations.
YES	Process the N.PERTURB input list to obtain perturbation factors for material densities, perform the perturbation calculation. The N.PERTURB list, if applicable, is processed directly by RACER3D. The general form is:

N.PERTURB = MATERIAL *c*1 FACTOR *f*1, MATERIAL *c*2 FACTOR *f*2, etc.

where *c*1, *c*2, etc. are the names of material compositions which are actually used in the problem (and may include tuples, if appropriate), and *f*1, *f*2, etc. are non-zero multipliers to be applied to all nuclide densities in the base compositions. The perturbed compositions must be the names of explicitly used materials; compositions which comprise only a portion of another composition cannot be perturbed.

DELTAPF, <i>x</i>	{.5} The parameter to be used in determining the minimum mean-free path for grids in delta-tracking edit-groups. Meaningful only when "PERTURB, YES" is selected. "x" should be chosen such that $0 < x < 1$. The value .5 is currently recommended.
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