LA-UR-11-04363

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Intended for: International Conference on Nuclear Criticality (ICNC 2011)
September 19-22, 2011
Edinburgh, UK

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Form 836 (7/06)

OVERVIEW OF MCNP6 CAPABILITIES FOR CRITICALITY ACCIDENT IMPACT ASSESSMENT AND ALARM SYSTEM DESIGN

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ABSTRACT

The MCNP6 Monte Carlo software package involves several capabilities that are of interest to designers of criticality accident alarm systems. These capabilities are useful in the areas of source characterization from a criticality accident, radiation transport and dose assessment, and detector calculations. MCNP6 comes with verification and validation suites containing problems that are relevant to these calculations. The development team also gives advanced criticality courses that can, by request, feature lecture material to explain how MCNP6 can be used in this area.

Key Words: Monte Carlo, radiation transport, detectors, validation, training

1. INTRODUCTION

MCNP is designed to be a general-purpose Monte Carlo radiation transport software package. The package has a development history spanning decades and is still undergoing development. Version 5 of MCNP, or MCNP5 [1], featured a rewrite to adhere to more modern software development practices (e.g., the Fortran 90 standard), and has more recently been largely funded by the US Department of Energy Nuclear Criticality Safety Program (NCSP). Version 6 of MCNP, or MCNP6 [2], is slated for general release in the next year (an initial beta release to a very limited set of users is currently available) and contains a broad spectrum of new features, many of which are inherited from MCNPX [3], a derivative software project that is being merged into the main MCNP code base.

Recently, many engineers within the NCSP have been tasked with the design of criticality accident alarm systems (CAAS) [4, 5] for new or design changes to existing facilities. MCNP6 contains many legacy and new features that may be of interest to CAAS designers. Namely, the topics of interest are the characterization of the source, the transport of neutron and gamma radiation throughout a facility, and the detection of that radiation. Also, the MCNP development team devotes effort to validation, and some of these are relevant to the CAAS designer.

2. TRANSPORT, DOSE, & DETECTION CAPABILITIES

2.1. Source Characterization

Modeling the source from a criticality accident is, in general, a very difficult problem and MCNP6 is most limited in this phase because it only solves the linear-transport equation with no feedback. Often times, this problem can be avoided altogether because the intensity of the source is prescribed with two limits: a “minimum accident of concern” and a “maximum credible accident”. The minimum accident of concern is typically defined as the accident of minimum strength the produces some biological dose at a certain distance away, and is the minimum accident an alarm system must detect. The maximum credible accident is usually defined by some regulatory requirement determined from conservative estimates based upon previous accidents, applications of point-kinetics models, or experimental measurements from pulsed assemblies. The maximum credible accident represents the worst-case impact that must be designed for as well as an upper survivability limit for a CAAS.

In cases where a more realistic characterization is required, the intensity of the source from a criticality accident can be computed independently using methods discussed extensively in the literature [6–9]. Typically, simple point-kinetics models are used that require parameters such as the effective delayed neutron fraction and the neutron generation time. These can be obtained using the adjoint-weighted tally feature [10–12], in MCNP6 (first released in MCNP5-1.60 [13]). As for spatial characterization, typically point sources or volumetric sources are sufficient. In MCNP6, neutrons and gammas from the source may now be specified together, unlike MCNP5 (this capability was first implemented in MCNPX 2.5.0 [14]).

Often times, intrinsic sources are present in a criticality facility (e.g., cobalt-60 calibration sources) and the CAAS designer must ensure that these intrinsic sources do not cause false alarms. To assist with this MCNP6 has spontaneous fission and spontaneous gamma emission sources (first implemented in MCNPX 2.5.0 [15]).

2.2. Radiation Transport & Dose Assessment

Once the source is obtained from other means, the radiation needs to be transported throughout the system to evaluate doses and detector responses. The first consideration is the constuction of the facility geometry. This can be done using the combinatoral-solid geometry routines available in all versions of MCNP; MCNP6, however provides a new unstructured mesh feature [16, 17] that may be a convenient geometric modeling alternative for many users. The MCNP6 unstructured mesh capability uses a geometry file in the ABAQUS format [18], which may be produced by that or many other computed-aided engineering programs. Should such models of a facility, or important components within a facility be available, it may save a CAAS engineer time by incorporating them into the MCNP geometry.

For neutron and photon transport physics in this application, typically the default transport features are sufficient. Unless comparison must be done to previous calculations using older data, it is recommended to use the newest available nuclear data set, which, at the time of this writing, is currently ENDF/B-VII.0 [19]. For dose assessment, typically higher energy neutrons and photons tend to be the most relevant. When modeling neutron detectors, some thermal physics may be important and use of $S(\alpha,\beta)$ laws are recommended where appropriate (such as modeling polyethylene surrounding a Bonner sphere).

The calculation of global dose from an accident, to either do triage, impact assessment, or alarm placement is best done via the application of mesh tallies. A mesh tally is a structured (not necessarily regular) grid (typically Cartesian, but cylindrical, for MCNP5 and MCNPX style, and spherical, for MCNPX style only, options are available) of flux tallies that is overlaid on top of the problem. Both MCNP5 and MCNPX implemented mesh tallies differently and have slightly different feature scopes and input formats. Typically, the features in the MCNP5-style mesh tallies (the FMESH card) are more applicable for these types of calculations, and can be easily connected with energy-dependent dose/response functions.

Dose/response functions can be specified using the DE and DF cards in conjunction with the FMESH. During particle transport, the values of the dose/response function act as a tally multiplier that is interpolated based on the energy grid (combinations of linear and logarithmic interpolation are available). For biological or absorbed dose, MCNP6 has several commonly used dose functions (currently available in MCNPX) by use of the DFACT card, or the user may provide his or her own. Dose functions are also useful to correct tally responses with experimentally measured detector efficiencies.

Since neutron and photon populations from a criticality accident are assumed to be high (otherwise they would not be of concern to human health), most CAAS calculations depend only upon mean-value quantities. It is therefore appropriate in many circumstances to employ variance reduction techniques with the intent to accelerate the statistical convergence of tallies. The choice of variance reduction techniques depends upon the application, and three techniques are discussed: weight-windows, forced collisions, and DXTRAN spheres.

2.2.1. Weight windows

The use of weight windows is a popular technique for many classes of fixed-source problems. Weight windows are a means where the numerical weight of the particle is controlled in ways that preserve the expected score of all tallies while hopefully reducing the distribution of weight and therefore the variance of the scores. Similar to mesh tallies, the space is subdivided by a mesh and each mesh element is assigned a lower weight-window bound – in MCNP, the upper weight-window bound is a global constant factor multiplied by the lower bound – that is inversely proportional to the importance of that region with respect to the tally of interest. Upon entering a region, if a particle has a weight higher than the upper weight-window bound, then that indicates that track is important and it is split into multiple copies such that the weight of each particle is within the weight-window. Conversely, if the particle weight is below the lower weight-window bound, then this indicates that the track is not so important and it undergoes Russian roulette, a process where only of a fraction of the particles continue with a higher weight such that the average weight is preserved.

It is rarely practical for a human to understand the problem in enough detail so that he or she may assign the lower weight-window bounds, and therefore some automation is required. MCNP has a statistical weight-window generator [20] (available since the 1980's) that will attempt to optimize toward transporting particles toward an individual tally. For modeling the response of an individual detector in a facility, the long-standing generator will probably be sufficient.

Optimizing to multiple or global responses is less straightforward and has been the subject of much research for over a decade [21–26] and have been shown to be effective at significantly accelerating the convergence in CAAS-type problems [27, 28]. Many of these approaches involve a so-called hybrid method that couples Monte Carlo and deterministic packages together. MCNP6 has a capability that is under development for linking with PARTISN [29], a discrete ordinates radiation transport solver from Los Alamos National Laboratory (LANL), to generate adjoint (importance) functions that are converted into lower weight-window bounds. Should a deterministic method not be desirable, an iterative Monte-Carlo only method for generating global biasing functions for weight windows [24] is under development, but will probably not be in the initial MCNP6 release. In addition there has been research dedicated toward assessing the statistical convergence of global tallies [30], in addition to possible measures of efficiency for various global biasing parameter sets [31].

2.2.2. Forced collisions & DXTRAN spheres

Forced collisions and DXTRAN spheres are variance reduction techniques that have been present in MCNP since the early days, and these techniques are particularly useful for detector-type calculations in CAAS problems. The forced collision technique does as it says to attempt to increase the collision rate in cells. Typically this technique is most effective in low-collision media such as air. In the simulation, MCNP separates the particle into a collided and an uncollided (transmitted) part; the weights of both parts are assigned to preserve the expected value of tally scores.

Forced collisions are particularly useful when used in conjunction with DXTRAN spheres. The DXTRAN technique is perhaps the least intuitive variance reduction technique in MCNP; however, they are very useful for many applications such as CAAS design because they are capable of angular biasing at collisions forcing more particles to reach (often small) regions of interest, such as a detector. At each collision (including forced collisions), the particle is broken into two particles, a DXTRAN and non-DXTRAN particle. The DXTRAN particle is transported deterministically without collision to the surface on some defined sphere, typically containing a detector geometry. The non-DXTRAN particle continues normally, but is terminated if it reaches the surface of the DXTRAN sphere – this is done to preserve expected tally scores. The use of a DXTRAN sphere around CAAS detectors and forced collisions throughout the geometry can be an effective means to get particles to reach the detector at a significantly higher rate in the Monte Carlo simulation than they would in the analog case. If multiple DXTRAN spheres are used, weight control via weight windows are strongly recommended, and the use of weight windows is generally a good idea anyway.

The new feature in MCNP6 that may be useful to some CAAS designers is the ability to nest DXTRAN spheres [32]. This is useful when detectors are nearby each other and it can serve as a way to pull particles toward regions of interest in a cascading fashion.

2.3. Detector Modeling

MCNP6 has many features available for the modeling of detectors, especially those incorporated from MCNPX. Many of these involve features pertaining to spectra and coincidence counting for applications involving material detection, and have little relevance to CAAS applications where fluences are typically very high. For this reason, most of the MCNP5 features should be sufficient for most CAAS calculations.

Detectors may be modeled explicitly in the problem geometry to preserve as much fidelity as possible, or they may be treated approximately as a point. While the former is most likely to be the most accurate, using point approximations allows for major improvements in calculation efficiency. For explicit modeling, the detector geometry and materials are placed into the geometry along with appropriate energy deposition (F6 type) tallies – the MCNP6 unstructured mesh capability may be useful here if ABAQUS models of the detectors are available or can be created without much effort. Getting sufficient scores to the tally can be very difficult because usually the detector is very small relative to the entire geometry, so significant variance reduction will probably be required. The use of dose/response functions may still be required to capture detector efficiency, since various complicating factors such as dead time leads to not all energy deposited in the detector to be registered by the signal detection equipment.

Point approximations can be useful if the geometric details are unimportant and the detector itself has little impact on the overall particle transport, as is often the case. This makes use of the flux at a point (F5 type) tallies, that accrue scores each collision via straight-line attenuation from the point of collision to the detector. Typically, the use of a point detector tally yields statistically significant results more efficiently than if the explicit model is used. CAAS designers, however, should not be misled to believe that point approximations necessarily require any less effort to ensure accuracy is preserved. Appropriate tally multipliers must be applied to preserve energy deposition rates. A dose/response function is almost surely required to account for energy-dependent detector efficiencies (an advantage of explicit modeling is that it can capture finite size effects). MCNP6 can be used to calculate some effects of detector efficiency by using an explicit model in an experimental setup and computing the actual energy deposition relative to the theoretical amount deposited.

When using point detectors, MCNP5 and MCNPX use a post-collision next event estimator. In other words, the attenuation calculation is performed after the specific reaction has been chosen. MCNP6 features a pre-collision next event estimator that accrues a contribution from each type of possible reaction that may occur in the collision. The sampling of all reaction types typically improves the scoring efficiency significantly for most photon problems, and has smaller gains for neutron problems.

Specrta may also be desired for some applications. In this case, it is important to use Gaussian energy broadening to capture the effects of finite resolution of the detector, especially for photons in the 100 keV range [33–35]. This feature has been available in MCNP5 and is also available in MCNP6.

3. VERIFICATION, VALIDATION & TRAINING EFFORTS

For software to be useful, it must be verified and validated. Verification involves ensuring the methods within the software are performing as intended. Validation is comparing computational results with experimental measurements to ensure the software and its associated data can adequately address the problems of interest to a user. The MCNP development team performs verification and validation; however, the validation is quite broad and usually does not address any specific application with any depth, so the end users must still perform validation for their problems of interest.

The MCNP development team also gives training to users in both broad introductory and topic-specific advanced courses. Relevant efforts related to the training of users for CAAS designers is discussed.

3.1. Verification & Validation Test Suites

MCNP6 has several suites for verifying and validating the software and its nuclear data that are of interest to a CAAS designer. Three verification suites that are of particular interest are the Verification K-Effective [36], the Kobayashi benchmarks [37], and the Neutron Generation Time [12] suites. The validation suites that are of relevance to the CAAS designer are the Expanded Criticality [38], Rossi-α [39], and Shielding [40] validation suites.

3.1.1. "Verification K-Effective" suite

The Verification K-Effective suite involves 75 simplified, one- or multi-group problems where k has analytic solutions. MCNP6 is run on these problems to show that tracking, collision, and criticality routines are working correctly. For the CAAS designer, these are important for showing that MCNP6 can perform the assessment of the types of accidents that can credibly occur.

3.1.2. "Kobayashi" verification suite

The "Kobayashi benchmarks" are a set of 3-D, mono-energetic benchmark problems consisting of simple geometries containing void regions. There are three configurations, and each set is run as a pure absorber and with scattering. The pure absorber cases have exact solutions available, and comparison is with them. Those with scattering are compared to very tightly converged calculations with the MVP Monte Carlo software package. Overall, 136 different flux values are estimated at different points with point detectors throughout the problems, and comparisons are performed. This set demonstrates the tracking and point detector capabilities of MCNP6 in duct-streaming type geometries that are of interest to the CAAS designer.

3.1.3. "Neutron Generation Time" verification suite

This suite compares MCNP computed values with mono-energetic and multigroup values of the neutron generation time Λ in infinite and finite media. For infinite media, analytic solutions are available [41]. For the finite media, forward and adjoint fluxes from PARTISN are used to generate reference values. This suite is of interest to those CAAS designers desiring a characterization of a source intensity using point-kinetics models, since it shows that the adjoint weighting methodology is implemented correctly.

3.1.4. "Expanded Criticality" validation suite

The Expanded Criticality validation suite contains 119 benchmarks found in the International Handbook of Evaluated Criticality Safety Benchmark Experiments [42] (ICSBEP). This suite is used to see how well MCNP6 and a particular data set can predict k measured by an experiment. It is also used by the nuclear data developers of ENDF in the development of nuclear datasets. While this suite is generally more interesting for traditional criticality safety applications, it does have relevance to the CAAS designer because it can provide information about the performance of nuclear data for particular materials and isotopes of interest such as water, uranium solutions, air, etc.

3.1.5. "Rossi-α" validation suite

This suite contains 13 benchmarks from the ICSBEP that have measured values of Rossi-α at delayed critical and is used to show how well MCNP6 can compute this quantity. Why this matters to a CAAS designer is that Rossi-α is the ratio of the effective delayed neutron fraction β and the neutron generation time Λ. Both these independent quantities are of importance for source intensity characterization from a criticality accident.

3.1.6. "Shielding" validation suite

The Shielding validation suite contains about a dozen problems designed to test MCNP6's (with nuclear data) capability to predict neutron transport and photon production and transport through various materials such as air, water, concrete, iron, lead, etc. This suite is of particular relevance to CAAS designers because the design problems they are similar to those doing shield design. This suite is currently being overhauled to provide a greater coverage of applications to the CAAS designer.

3.2. MCNP Training for CAAS Designers

The MCNP development team runs courses on general and specific topics. Some of the specific topics include criticality, variance reduction, and health physics/detection: all of which may be useful to a CAAS designer in some way. The NCSP sponsors on-site criticality courses for MCNP at US DOE/NNSA facilities, and the MCNP developers customize their course material based upon the demand of the students at each site.

The course performed in spring of 2011 at the Y-12 National Security Complex involved, by request, a new lecture specifically for CAAS designers; the title of this lecture is "Tallies and Shielding Calculations for Criticality Safety" and spans an entire day. The first half of the lecture involves basic problem of a 1-D multi-layer shield and discusses the topics of fixed sources, tallies of fluxes, reaction rates, and spectra, use of dose functions, tally plotting, and basic variance reduction techniques. The second half of the lecture focuses on a simple, but realistic model of a criticality accident in an experimental facility. The topics are mesh tallies, more advanced variance reduction techniques (the weight-window generator, forced collisions, and DXTRAN spheres), and basics on modeling detectors.

4. SUMMARY

MCNP6 involves the merger of MCNP5 and MCNPX and new features found in neither. Many of these features are particularly useful for CAAS designers attempting to characterize a source, model radiation transport through a facility to measure dose, and to model detectors. The MCNP development team provides six verification and validation suites that are of particular interest to

CAAS designers, and, for those within the NCSP at DOE/NNSA facilities, offers training courses that can be custom tailored to CAAS designers.

New features are continuously being developed in MCNP6, and some of these may be applicable to CAAS designers. The MCNP development team has, as part of its design practices, the need to perform verification and validation on new features to ensure MCNP6 is a quality product for its users. To make users aware of new and relevant features, the development team also conducts training courses at LANL for general attendance, and site-specific classes for those in the NCSP at DOE/NNSA facilities.

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