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**Title:**

**AN INTRODUCTION TO MONK7**

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## SUMMARY

MONK is a Monte Carlo neutronics computer software package written to assist in the study of criticality safety problems. The release of MONK7A is the culmination of a major programme of work which has comprised both the development/enhancement of the package functionality and the re-engineering of the software structure. This paper describes the additions and modifications that distinguish MONK7 from its predecessor together with an overview of the new supporting graphical tool VISTA. Plans for future development of the MONK code are also outlined.

## INTRODUCTION

MONK [1] is a Monte Carlo neutronics computer software package written to assist in the study of criticality safety problems. MONK originated from a code called GEM, which came out of the post-war nuclear weapons programme in the United Kingdom. The first appearance of MONK was about thirty years ago, and the main software user benefits have been retained to this day, although they have been considerably enhanced in the intervening years. These are:

- geometry modelling - the MONK geometry modelling package is the most easy-to-use and flexible package available in any widely-used Monte Carlo particle transport code
- nuclear data/collision processing - the use by MONK of continuous energy modelling has significant benefits in terms of accuracy and ease-of-use when compared with multi-group methods
- user interface - MONK has an easy-to-use input syntax supported by wide-ranging validation data, user-oriented documentation and intelligible output syntax

MONK is widely used in both design environments and in support of regulatory license submissions and has been accepted by the USNRC following the submission of a Topical Report. Until now, the most recent period of development was stimulated by the expansion of the UK reprocessing industry in the 1980's, particularly the design and construction of the Thermal Oxide Reprocessing Plant (THORP) by British Nuclear Fuels plc (BNFL), and resulted in the production of MONK6. MONK7A is the culmination of further development designed principally to bring MONK into a more modern software environment. This paper describes MONK7A by comparing the features it contains with those of its immediate predecessor, MONK6.

## BACKGROUND

MONK is distributed and actively supported in use by the ANSWERS Software Service of AEA Technology. As a commercial product, any strategic development of the software package needs to take account of both current and future customer requirements. In order to accomplish this for MONK7, the development was performed within a collaboration between AEA and BNFL in order to ensure that the finished product was both acceptable to the user community and commercially viable.

One significant consequence of this is that the major features and options of MONK6 have been retained in MONK7A in a familiar form, although some minor options have not been carried forward. In addition the new features of MONK7A have been incorporated in a consistent manner in order to enable a seamless transition to be made between the old and the new. These changes are summarised in this document, together with the modifications to the code user image that have occurred.

The release of MONK6A in 1987 was the culmination of the original MONK6 development project which started in 1979. Some minor enhancements then followed which led to the release of MONK6B in 1989. Subsequently, and in recognition of the inherent problems that would limit the future development possibilities for MONK, a major reconstruction exercise was undertaken to bring MONK into a more modern software environment. This development (and currently on-going development) has been performed by the collaboration within a Quality Management System accredited to ISO 9001.

Internally, MONK7A is a significantly different package than MONK6, with large sections of the software having been re-written or replaced. These activities have been performed for two principal purposes:

- to install MONK in a more modern programming environment (the so-called MCANO Modular Code Scheme [2]), to facilitate future development and maintenance

- to enable MONK and the Monte Carlo general particle transport software package MCBEND [3] to share facilities where practicable, so that the use of Monte Carlo particle transport development resources can be optimised

A further objective of the work was to ensure that adequate back-compatibility was provided so that MONK users could take as much advantage as was reasonably possible of their invested effort in existing code models. Inevitably, certain compromises have had to be reached, but it is believed that the resulting software package will prove an adequate and acceptable replacement for MONK6, and a suitable vehicle for onward development.

## OVERVIEW OF MONK7A

A large part of the MONK7 development programme has been concerned with combining the functionality of MCBEND and MONK into a single modular code scheme and rationalising, wherever appropriate, the areas within the existing packages which overlapped. One of the main areas of activity has been the geometry package, where due to their separate development histories MONK and MCBEND have traditionally employed different specification formats and tracking routines. Some rationalisation was seen as being essential in this fundamental area if the full benefits of the MCANO code scheme were to be realised.

The rationalisation has lead to the production of a new geometry specification package (Fractal Geometry or FG), which combines the best features of the existing MONK and MCBEND facilities, yet maintains (for back-compatibility) the existing geometry user images of both packages. However, whatever format the user employs to specify the geometry, MONK will convert the data and perform the geometry tracking using the FG package, which is considerably more efficient than its equivalent in either MCBEND or MONK.

A further major change is the incorporation of a new thermalisation treatment based on a superior physical model for hydrogen when bound in water and poly-carbons. To access the new treatment requires the specification of different identifiers for the nuclides involved. Note that the MONK6 treatment has been retained as an option for back-compatibility purposes.

MONK7A contains a new starting source option to replace many of those contained in MONK6B. Here it was deemed necessary to deviate from strict back-compatibility in order to produce the simplified package being sought, although simple approximations to many of the MONK6B source options is automatically provided for in MONK7A. The changes to input specifications to use the new option explicitly are relatively minor.

It should be noted that MONK7A has two distinct user images:

- that of MONK6: for back-compatibility with existing models

- that of MCANO: intended for new work and the style upon which future development will be based.

It is hoped that over a period of time the MCANO input will become the preferred option for all users as it retains all the best features of the MONK6 format, yet removes some of the minor irritations that have been observed over the years. Recent experience in introducing MONK7 to new users has supported the claim that the novice user can be efficiently employing the code to solve real application problems in only three or four days. In addition, use of the MCANO syntax provides direct compatibility between MONK and MCBEND and enables input specifications and modelling expertise to be readily transferred between the two application areas.

The output from MONK7A is another area where major changes have occurred, although little of significance has been lost. The input interpretation summary has been completely overhauled to produce a common format for MONK and MCBEND; the opportunity has been taken to tidy up the layout and remove redundant information. The results section has changed rather less in content and format (as requested by the majority of users). However some general tidying and miscellaneous improvements have been performed and greater user control over what is printed is now available.

Finally, the MONK user guide has been comprehensively revised as follows:

- production of an easy-to-follow input description in the form of flowcharts and associated notes

- provision of a wide-range of annotated realistic application examples

- a general geometry modelling description together with advice for complex situations

- a summary of the MONK validation database

Note that the MONK user guide is a controlled document subject to review and update as required, for example to include additional data arising from the on-going MONK validation project. This ensures that users are employing up-to-date documentation to support their application of safety-related software.

# CODE FUNCTIONALITY ENHANCEMENTS

## Nuclear Data Library

One of the major developments for MONK7A has been the production of a new thermalisation modelling treatment employing up-to-date hydrogen scattering data from the JEF library. The new treatment has been designed to replace the MONK6 treatment, with the provision of collision models and data for hydrogen in water and hydrogen in poly-carbons.

The new treatment includes $S(\alpha,\beta)$ functions for use in modelling inelastic thermal scattering as well as a model for incoherent elastic scattering, which is particularly important for hydrogen in polythene.

The effects on k-effective of the new treatment have been shown to be small for many situations, but the extra physical realism will provide greater intrinsic accuracy. Note that the existing MONK6 thermalisation treatment for hydrogen-in-water has been retained for full back-compatibility. The remaining nuclides in the continuous energy nuclear data library are unchanged, although the library has been extended by the addition of some further fission product nuclides taken from the JEF library.

The time-scale for the adoption of a new library completely derived from JEF data is currently being investigated [4] as part of a widespread benchmarking programme for the JEF2.2 library. For the time being all validation analyses performed as part of the AEA/BNFL MONK validation database enhancement project [5] are being analysed with the current MONK7A library and the pre-release JEF-based library, in order to be able to plan such a move.

## Geometry Modelling

A review of the geometry modelling requirements for Monte Carlo modelling was performed as a prelude to further development of MONK [6]. Having considered the major options of existing methods, the new Fractal Geometry (FG) system has been developed satisfying the requirements for an efficient, powerful and user-friendly geometry package. The FG system is included in MONK7A and can be summarised as follows:

- The input stage - The geometry uses solid bodies for its basic construction units with the model constructed as a set of parts which may be hierarchic to any level (see Figure 1). The bodies in each part are defined using a co-ordinate system local to that part and can be freely oriented within the part. The zones in a part are the insides of single bodies (the MONK nest and cluster concepts) or the differences and intersections of two or more bodies (general body combination).

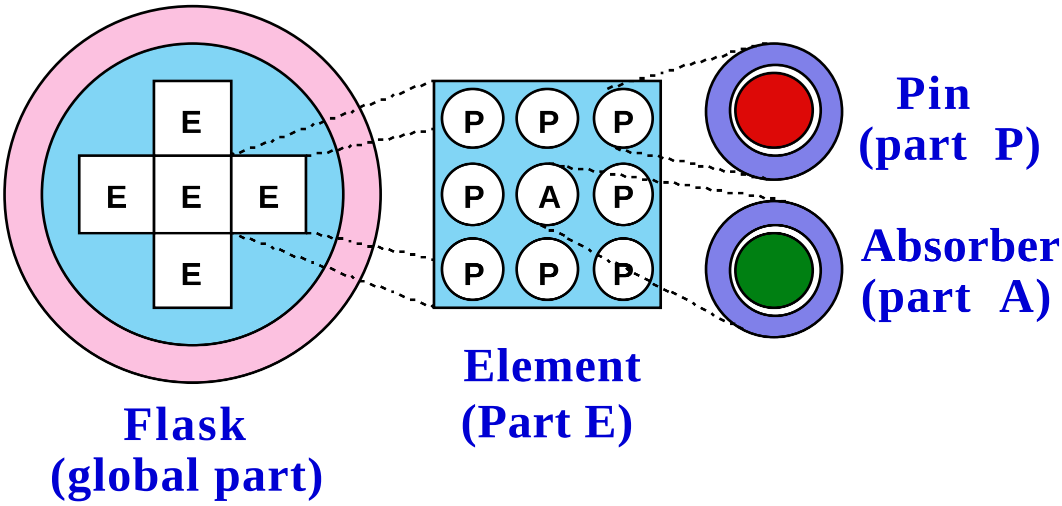

Figure 1 - Example of Part Hierarchy

Zones can contain single materials, complete subsidiary parts or one of the unique Woodcock tracking geometries (within these geometries conventional particle tracking is replaced by a cascade process which enables geometry descriptions of almost limitless complexity to be described - Figure 2 shows the MONK screw-feeder Woodcock tracking option)

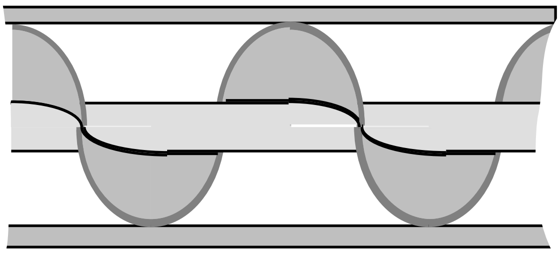

Figure 2 - Example of Woodcock Tracking Geometry

- Intermediate processing - The code expands the input geometric data to form a global model in which each body definition is translated and rotated to an absolute location. The bodies are converted to a surface system for robust and efficient tracking. Coincident surfaces are identified and discarded during this process. A zone relationship map is prepared to allow the code to follow the logic of the input part structure.

- Tracking - The final model is based on zones bounded by surfaces and the map of neighbouring zones will be learnt as the tracking process continues. Woodcock tracking may be used in any zone.

Fractal Geometry also includes additional bodies from the set available in previous versions of MONK as the ellipsoid and infinite plane are now available. In addition further Woodcock tracking hole geometries have been developed, namely the 'rzmesh' and 'xyzmesh' types.

An advantage of Fractal Geometry is its ability to absorb the user image of established systems. A conventional MCBEND model is achieved by having a global part with no daughter parts. Additional bodies corresponding to single surfaces may be introduced to simulate a surface geometry input. The standard structures of the MONK geometry exist as a sub-set of permitted FG structures. By this means acceptable back-compatibility with existing models can be provided while at the same time providing a common way forward across different application areas. This will provide increased flexibility to user groups as well as reduced overheads associated with training and maintenance of expertise.

## Starting Source Options

MONK6 contains a wide range of starting source options to meet the requirements of criticality calculations. Some of these options were developed some time ago to address what were then perceived to be sampling/settling problems. Following the theoretical analysis of Monte Carlo eigenvalue algorithms which led to the development of the superhistory tracking algorithm [7], a greater understanding of the sampling/settling process was achieved. This led to a greater awareness of the parameters that can cause problems and a reduced need for fine detail spatial starting source distributions.

The development of MONK7A was a convenient time to rationalise the MONK source options, particularly taking account of the very wide range of facilities inherited in the MCANO code scheme from MCBEND.

## Geometry Visualisation

Companion packages to MONK exist called VISAGE and VISTA which are used to produce pictures of the geometry model. These are produced interactively on a high-resolution computer monitor in two or three dimensions (VISAGE and VISTA respectively).

VISAGE is a high-resolution mouse and menu driven graphical tool for the interactive generation, display and manipulation of two-dimensional slices through the geometry specification. VISAGE has been implemented in C and uses the X-Windows and OSF/Motif tool-kits and hence is highly portable. VISAGE images are produced using the geometry tracking routines of MONK and so are a genuine indication of the geometry seen by the modelling packages themselves.

VISTA performs the interactive generation, display and manipulation of three-dimensional images by two independent means. Firstly an option exploits the portability of X-Windows, OSF/Motif and PHIGS, and the power of modern workstations, to give three-dimensional wire-frame based displays of the geometry specification. PHIGS is an international standard for three-dimensional computer graphics which has been implemented on many of the major computers currently in use. The option provides a range of visualisation options including cutting planes, sections and shading.

The user image for VISTA employs the same mouse/menu environment as VISAGE and has a range of viewing and manipulation options. The use of PHIGS means that the images produced from this part of VISTA are not derived using the geometry tracking routines of MONK. However the power and versatility of PHIGS enables a comprehensive interactive display package to be produced permitting rapid visualisation and manipulation of the images.

The second component of the VISTA package is the generation, display and manipulation of three-dimensional rendered images using particle tracking techniques. Here the images are produced using the geometry tracking routines of MONK so the images produced are a genuine indication of the geometry seen by the modelling codes themselves. X-Windows and OSF/Motif have again been employed to provide a similar user image to that of VISAGE. The images are produced using a simulated optical ray tracing algorithm which requires the tracking of rays from a viewing plane into the geometry model until a visible zone boundary is reached.

Although this component of the VISTA package is slower in execution compared with the wire-frame generation component, it does provide a valuable additional verification function due to its direct link with the geometry tracking routines of the modelling codes. In combination, VISAGE and VISTA provide a comprehensive set of geometry verification tools to accompany the geometry package of MONK. An example three-dimensional VISTA image is shown in Figure 3.

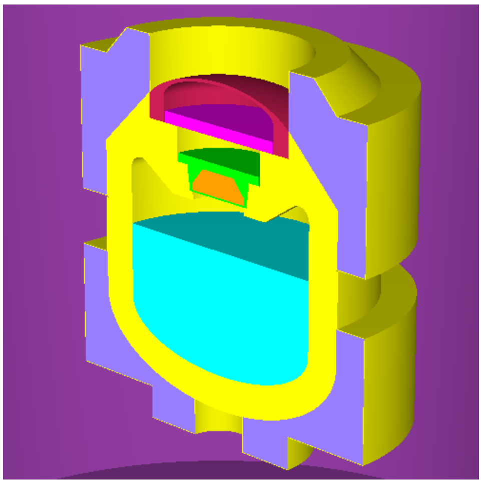

Figure 3 - VISTA Image of MONK Model

## VALIDATION

The on-going validation programme for MONK6B comprising detailed experimental re-evaluations [5] has now switched to using MONK7A following the new code's release. The additional validation and integral testing that has been performed for MONK7A prior to its release comprised the following five stages:

### Correction Of MONK6B Errors

All reported errors contained in the MONK6 observation file were investigated. Note that due to the replacement of major sections of the coding and the removal of certain options many of the MONK6B observations are not applicable to MONK7A. For those that do apply, a suitable test case was run to check that the error has been corrected.

### MONK6B Core Validation Set (MONK6 User Image)

The MONK6B core set of validation cases were run with MONK7A with the following objectives:

- To test the acceptability of MONK6 input specifications to MONK7A over a wide range of problems
- To test the MONK7A output tables for a wide range of problems
- To test the values of k-effective calculated by MONK7A. Although the coding has been extensively changed, one option is for MONK7A is to use the same nuclear data as MONK6B and therefore produce statistically indistinguishable results.

### MONK6B Core Validation Set (New Thermal Treatment)

Although direct back-compatibility with the MONK6B nuclear data library is provided by MONK7A, the recommended option is to employ the new thermal treatment. For the MONK user this means employing the new JEF-based bound hydrogen data for hydrogen in water and hydrogen in polycarbon as appropriate. All suitable cases from the MONK6B core set were re-specified to use the new data and re-run to determine the effect of the new thermal treatment on the calculated values of k-effective for a range of problems. For many problems the new treatment resulted in little difference to the calculated value of k-effective.

### MONK6B Core Validation Set (MCANO User Image)

A representative sample of the input specifications were converted into the MCANO user image. These were re-run with the objective of confirming the compatibility of the two user images.

### New MONK Validation Database

The MONK validation database has undergone a major overhaul comprising the re-evaluation of selected critical experiments. All such experiments studied to date have been re-specified and re-run using MONK7A together with the new thermal treatment. These calculations are forming the basis of the MONK7A validation database which is being actively expanded as more experiments are studied.

### In Service Use Prior to Release

A six-month field testing period for MONK7A was carried out by AEA and BNFL user groups. Users in both organisations were encouraged to employ the software alongside MONK6B for as many of their on-going projects as possible and report their observations. The objective of this stage of the testing was to expose the new software to a wider range of problems and users in order to assess its reliability and robustness and to increase user confidence prior to its recommendation for use. Due to the enthusiastic feedback provided by the user groups this part of the testing added greatly to the quality of the issued product.

## APPLICATIONS

During its long history MONK has been used in support of a wide range of industry projects covering the complete nuclear fuel cycle. To identify the reasons that this has been possible, we can refer back to the key software attributes that were highlighted in the introduction.

- geometry modelling - the accuracy of the MONK geometry modelling package enables plant items to be realistically modelled, avoiding the approximations that are required with other packages. This can lead to increased operator efficiency and flexibility, without in any way jeopardising safety.

- nuclear data/collision processing - the use of continuous energy modelling means that MONK can be employed with confidence across the full range of applications with the knowledge that the accuracy of the code is closely tied to the accuracy of the under-lying nuclear data. This avoids the inherent additional uncertainties present for the use of multi-group methods.

- user interface - the ease-of-use of the software together with the supporting validation data and documentation enables MONK to genuinely fill the role of an analytical tool, that can be quickly mastered and efficiently used to tackle the real safety and engineering problems.

Recent examples of the application of MONK to help solve major engineering and analysis problems include:

- design and commissioning of the new oxide fuel manufacturing facility by BNFL at Springfields to support the expansion of the company's LWR fuel element production business [8]

- on-going design of a commercial mixed oxide fuel manufacturing plant by BNFL at Sellafield to recycle plutonium for use in thermal reactors [9]

- optimisation of LWR fuel element storage and management by US utilities to increase capacity and improve efficiency

- investigation into long-term storage and disposal options for low and intermediate level waste within a deep repository [10]

## SOFTWARE MANAGEMENT AND FUTURE DEVELOPMENT

MONK7A is available through the ANSWERS Software Service of AEA Technology and has been commissioned on a wide range of computer hardware including mainframes, workstations and personal computers (PCs). The standard package issued by ANSWERS comprises: executable code modules, standard nuclear data library, sample problem inputs and outputs for implementation testing, hardware-specific installation guide, user guide and validation reports. Recent experience confirms that installation of MONK and completion of initial test cases can be accomplished in about two hours.

The ANSWERS Service offers a comprehensive user support package which includes maintenance, trouble-shooting and expert advice, as well as providing access to new code versions as they become available. In addition regular seminars and tailored training courses are held, including well-established hands-on workshops for those new to the code.

Development of MONK within the AEA/BNFL collaboration programme is continuing with the major effort currently being directed in two areas:

- Development of a new collision processing package aimed at making optimum use of modern nuclear data evaluations

- Benchmarking a nuclear data library based on JEF2.2 evaluations [4]

Other areas that are seeing development activity are: upgrade to material specification options; in-built multigroup collision processing for cross-checking; and calculation run-time sampling efficiency monitoring.

## CONCLUSIONS

A new version of the Monte Carlo criticality software package MONK has been produced, the first major upgrade for five years. A number of new facilities are available and a major programme of software re-engineering has been performed to prepare MONK for long-term future use, maintenance and development. A significant enhancement to the MONK geometry repertoire has been performed which has included additional modelling facilities and modern visualisation tools. Validation activity has been extended, so that the package is now distributed with a wide range of supporting experimental comparisons. Further major development is now under-way to maintain the level of progress and extend still further the capabilities and accuracy of the MONK package for continued use by the criticality safety community well into the next century.

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