

THE UNIFICATION OF MONK - EXTENDING THE MONTE CARLO HORIZON

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Abstract

The Monte Carlo criticality code MONK is a well-established and well-known tool for the solution of nuclear criticality safety problems. With an extensive track record of use in support of nuclear operations across the whole fuel cycle, the code provides sophisticated modelling capabilities in an easy-to use package. Development of the code continues however to meet new and emerging industry challenges as part of a collaborative venture between AEA Technology and BNFL - this collaboration has already produced MONK7 in 1994 as part of a major software re-engineering exercise in preparation for the major developments that have now followed. Less well-known than the criticality version MONK7 was the predominantly reactor physics variant MONK5W, utilising the renowned WIMS reactor physics nuclear data libraries. Although both codes originated from the same source in the 1970s, many years of independent development had led to the significant divergence of the two versions. Following the successful culmination of a three year development programme aimed at unification however, MONK8 is now available, bringing the full repertoire of both previous versions to the desktop in an integrated package. This paper will report on this major enhancement of the MONK software package, summarising the key developments that have taken place and their significance for the criticality analyst. The support of BNFL, Rolls Royce and Associates and British Energy during the course of this work is gratefully acknowledged.

Background

Early versions of the Monte Carlo criticality code MONK can be traced back well over thirty years and although modest developments subsequently took place, it was the needs of the UK reprocessing industry that led to the first major overhaul of the original code and resulted in the production of MONK6 in the late 1980's. This was followed by further enhancement and modernisation of the code and data (MONK7), together with the appearance of supporting productivity tools. In parallel with the above activity, a separate version of the code (MONK5W) was produced and subsequently enhanced specifically for reactor physics analyses, employing nuclear data from the WIMS [1] reactor physics suite of codes. Options specific to this reactor physics version of the code included a microscopic burnup treatment, an adjoint solution capability and point estimation of flux and fission rates.

The development and subsequent release of MONK7A was the culmination of a major renewal programme for the MONK criticality code. This comprised a comprehensive software re-engineering exercise to bring MONK into line with the successful modular system employed for the shielding code MCBEND [2]. This has provided customer and custodian benefits in terms of shared facilities and developments and more cost-effective and efficient maintenance. Version 7B was later released and included a range of extra features to extend the capabilities of the code.

Following the successful completion of an industry supported programme of unification, version 8A of MONK has recently been released and is the first version to provide the capability to perform both criticality and reactor physics calculations; thus MONK8 supersedes both MONK7 and MONK5W. A summary of the MONK versions and development paths is shown in Figure 1.

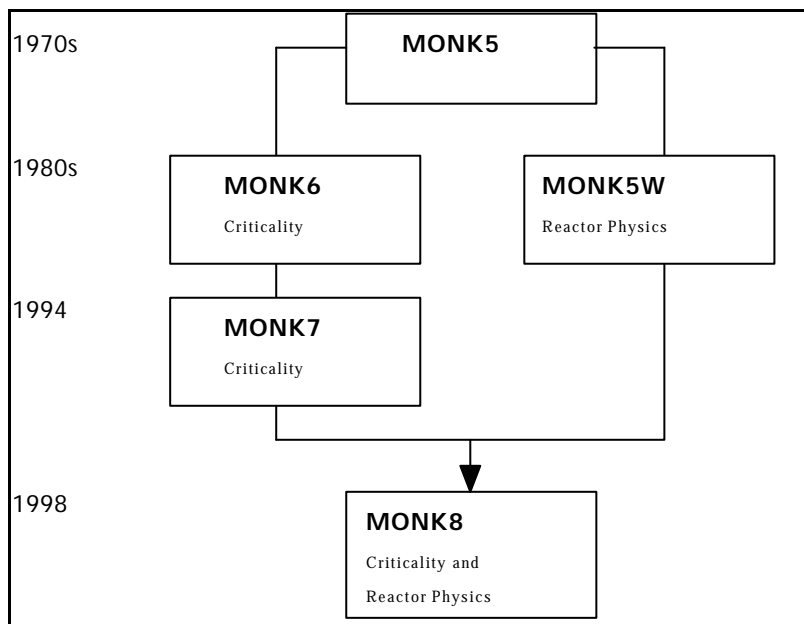


Figure 1 - Summary of Historic and Current MONK Code Versions

This paper starts by looking at the background to the MONK8 project and summarises the problems and issues that needed to be addressed. The majority of the rest of the paper then provides an introduction to the new code's capabilities as the horizons for practical Monte Carlo calculations become broader with the availability of the unique MONK criticality/reactor physics combination. A

look to the future beyond the current code version is also included. MONK is one of a number of modern physical modelling code packages distributed and actively supported in use by AEA Technology as part of its ANSWERS Software Service, with the MONK code development being performed by a collaboration comprising AEA Technology and BNFL.

Background to the MONK Unification Project

The first phase of the MONK unification project comprised a detailed review of the requirements of users of both predecessor codes (MONK7 and MONK5W). This industry consultation exercise resulted in the identification of the following principal benefits being desirable from the unification process:

- One Monte Carlo geometry specification package for all MONK users, entirely consistent with the package for the shielding code MCBEND
- Universal geometry visualisation tools for MONK and MCBEND
- Immediate access to enhanced capabilities - for example, the burnup option of MONK5W would be of immediate use to the wider MONK community due to its application in burnup credit
- New facilities arising from future development spin-off
- Reduced training requirements and increased staff flexibility
- More widespread code maintenance and development expertise
- Reduced costs for both the user and developer community

To provide these benefits, it was agreed that the following key objectives would guide the unification project itself:

- MONK7 would be used as the basis for the unification and extended incrementally by the addition of distinctive MONK5W facilities - as noted above, MONK7 was the result of a major renewal programme and the benefits from this could now be transferred to the unified code
- Phased releases of the emerging MONK8 code would be made to the industry group supporting the work so that experience with the new code could be achieved and feedback provided to influence later phases
- MONK would retain its place in the WIMS reactor physics code scheme in such a way that the same code version was employed in stand-alone MONK8 mode as was used within the WIMS Monte Carlo calculation route
- Previously separate Monte Carlo development teams would be merged to provide an integrated capability to support further maintenance and development of MONK and MCBEND

Following the establishment of the requirement, the MONK unification project proper started in April 1996. A team of four staff worked on the project over the next 27 months before MONK8A was released by the ANSWERS Software Service in June 1998. During the development cycle, three interim releases of MONK8 were made to BNFL and Rolls-Royce. Coupled with internal AEA Technology usage of the evolving code, this field trial usage of the package was very helpful in ensuring the successful conclusion and acceptability of the released code version. Further valuable features of the development cycle were the regular project meetings where developer and sponsoring representatives met to review progress and modify plans as required.

The starting point for the unification project was the 61,000 lines of MONK5W code and the 105,000 lines of MONK7. Working from the agreed MONK7 base, the final size of MONK8A was 174,000 lines, larger than the simple sum of the two independent codes (also noting that some parts of MONK5W were made redundant by this exercise). The increase in code size has largely come about by the improvements to the software engineering of the inherited MONK5W options in terms of code layout and design and internal commentary. In addition, the modular constructs of MONK7 possess modest overheads in terms of interface coding although the benefits of better functional and logical separation more than compensate.

In addition, there was a significant learning curve for the members of the project development team who were all familiar with one or other of the initial codes but not both. Common working practices needed to be developed and common understanding established as part of the general team building process. Also, in any change process there are likely to be human resource problems to be addressed and these too needed to be managed in parallel with the ambitious schedule for completing the MONK8 unification.

Finally of course, the project was completed, albeit with a two month over-run. A large amount of software has been reviewed, evaluated, understood, re-engineered, integrated, tested and documented and the final product is something of which those involved can feel justifiably proud. Now one year after release, the scale of what has been achieved is even more apparent as the code has been used by the wider MONK community to successfully solve criticality and reactor physics problems. If we review the perceived benefits of the unification process highlighted above, we can see to what extent they have (or will be) achieved:

- *One Monte Carlo geometry specification package for all MONK users, entirely consistent with the package for the shielding code MCBEND* - Achieved - A single geometry specification package is in use for the main UK Monte Carlo neutronics codes
- *Universal geometry visualisation tools for MONK and MCBEND* - Achieved - VISAGE and VISTA (see later in the paper) cover all MONK and MCBEND applications
- *Immediate access to enhanced capabilities* - Already achieved as expected for burnup credit and also in the use the hyperfine data library to cross-check WIMS library calculations
- *New facilities arising from future development spin-off* - Further geometry modelling developments are now underway that will benefit the wider community and the material specification library options are now being developed for WIMS data usage
- *Reduced training requirements and increased staff flexibility* - Already emerging for teams applying MONK to both criticality and reactor analyses
- *More widespread code maintenance and development expertise* - Already established during the unification project and this is now being built on
- *Reduced costs for both the user and developer community* - Arising from the above two items for the user and developer community respectively

MONK8 Overview

MONK8A is a markedly different package than either of its predecessor codes and is a worthy introduction to a new generation of the MONK code product. The specification for the scope of the new code version was assembled in the initial phase of the MONK unification project, where industry partners were consulted on their medium to long term requirements for the code. This was followed by

four phases of development, integration and rationalisation, with, at the end of each phase, a working version of MONK being produced for field trial usage. By this incremental means, continuing confidence of the partner organisations was maintained and valuable feedback was obtained by the development team on early usage of the new code as it was progressively rolled out.

The main new features of MONK8 compared with its criticality-only predecessor MONK7 are:

- *Reactor physics capability* - a suite of options that enable MONK to perform reactor physics calculations, including a microscopic depletion facility to perform calculation sequences following the changing fuel composition as a result of irradiation. This capability has already contributed to the development of a validated burnup credit analysis route.
- *Additional data library options* - choose from UKNDL, JEF2.2 and ENDF/B-VI hyperfine data and UKNDL, JEF2.2 (both WIMS format) and ENDF/B (SCALE format) broad group libraries all within the same code and using the same geometry model. Comprehensive cross-checking of key results has never been easier.
- *Splitting and Roulette* - importance sampling methods inherited from MCBEND to extend the scope of MONK to problems where preferential sampling is required to achieve acceptable code performance. Benchmarking small sample reactivity experiments is one example of the use of this well-established method in criticality analysis.
- *Enhanced usability options* - the ability to perform sequences of calculations concentrating on areas of interest together with other convenience tools to enable the user to optimise the use of available computer resources.
- *What else?* - lots more, including new geometry options, PC platform support, enhanced model visualisation tools, electronic user guide and an extended validation database.

Reactor Physics Calculations

The border-line between criticality and reactor physics has never been easy to define. Although traditionally two versions of MONK have existed to meet the needs of different user groups, as described above significant benefits have already emerged from the rationalisation of the teams working on the two codes and the synergy and development spin-off from the integration of on-going development programmes. More importantly, MONK8A has also already brought immediate benefits through to the analyst (for example burnup credit tools, cross-checking capabilities) and in the future one can expect to see additional cross-application developments arising from the new arrangements. Undoubtedly the major change for MONK8 is the presence of modern incarnations of the previously MONK5W-only reactor modelling options in an interface style entirely consistent with that pioneered in MONK7 for the criticality code users.

The principal new options included in MONK8A from this source are as follows:

- *WIMS Nuclear Data* - MONK8A now includes the capability to process and use WIMS group dependent nuclear data processed from the WIMS library. These data can be used as both conventional broad group pre-shielded cross sections in a defined group structure or as sub-group data.
- *Microscopic Burnup* - The MONK8A code includes a microscopic burn-up capability which will enable the code to treat whole core burn-up in small reactors. The burnup process requires special treatment because the irradiated fuel compositions vary with time and are dependent on their environment. In a real reactor core the material compositions change continuously with

time during burnup. To treat this process in MONK8 an extension of the methods used in deterministic calculations of burnup are used. Monte Carlo calculations are used to estimate the flux at a given time point and this flux is used to estimate the reaction rates of the materials in the problem. These reaction rates are then used to calculate the new material compositions by solving the depletion equations. Therefore the method adopted in MONK8A simulates the continuous change in material compositions by breaking down the process into discrete steps comprising a tracking phase followed by a burnup phase, then repeating these two phases until the required time period has been spanned.

- Output Options - The following output options have been included in MONK8A:
 - A collision density flux estimator in addition to the track length estimator
 - Migration area and buckling options for imposed leakage calculations and for comparisons with two-dimensional deterministic methods
 - Flux tilts and harmonic components for the estimation of peak power and for use in perturbation theory for estimating small reactivity changes
 - Reaction rates for burnup
- Adjoint Tracking - The calculation of the adjoint flux is required both for perturbation calculations and for point estimation of flux or reaction rates. The MONK8A method uses the same multigroup tracking techniques as the forward MONK solution but with the scattering and yield data transposed. In addition a bias function based on the normal flux may be input to improve the convergence of the calculation.
- Point Estimator - The calculation of flux or reaction rates at a point (or in a small volume) using the Monte Carlo technique can be both difficult and time consuming due to the low probability of tracks passing through the specified point or volume. The Point Estimator method was developed to solve this problem by making use of a kernel to calculate the required score, with the kernel being based on the adjoint function.
- Fixed Source Tracking - This option will calculate the multiplication and flux due to a fixed source in a problem with fissile materials. Multiple sources comprising any combination of points, lines, laminae and volumes can be used, each with a user specified relative probability of being sampled. In addition each of the sources can have either a user defined spectrum or the default fission spectrum. At the start of each stage the source is obtained from the source distribution and energy spectrum supplied by the user.

Data Library Options

MONK8 comes equipped with a range of standard data libraries that provide a host of inter-comparison and cross-checking possibilities, as well as providing linked Monte Carlo benchmarking capabilities for the WIMS deterministic methods. A summary of the options available to the code user is as follows (see also Figure 2):

- UKNDL-based hyperfine energy group library (8,220 groups) using a continuous energy/angle slowing down treatment. This has been the standard MONK criticality library for over ten years and due to its impressive performance is still in common use.
- JEF2.2-based hyperfine energy group library (13,193 groups) using a continuous energy/angle slowing down treatment. This is now being adopted by more and more MONK users following the completion of a wide-ranging benchmark programme comprising over five hundred experimental comparisons [3]. The modern evaluations represented here yield useful application benefits for MONK users in many situations.

- ENDF/B-VI-based hyperfine energy group library (13,193 groups) using a continuous energy/angle slowing down treatment. This library is a recent addition to the MONK repertoire and provides a useful additional route for the inter-comparison capabilities.
- UKNDL-based WIMS broad group library (69 groups) using a multigroup or sub-group treatment. This has been the standard WIMS library for thirteen years and has been so successful that it has been the benchmark against which subsequent library developments have been measured.
- JEF2.2-based WIMS broad group library (69 or 172 groups) using a multigroup or sub-group treatment. This is now emerging as the new WIMS standard library following a similar programme of benchmarking performed for the hyperfine equivalent library.
- SCALE data libraries. MONK includes a link module that provides access to standard SCALE libraries, typically the 44 and 238 group libraries for criticality applications.

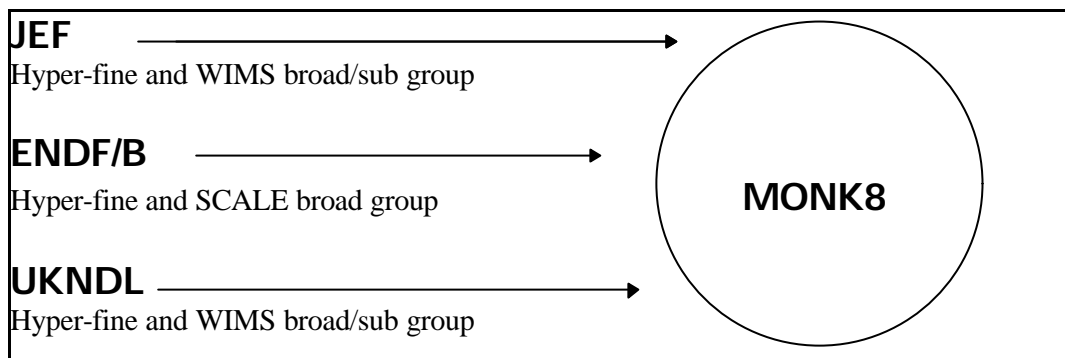


Figure 2 - Summary of the Nuclear Data Options for MONK8

Planned expansion in this area includes the production of a JENDL-based hyperfine library and an ENDF/B-VI-based WIMS library.

Splitting and Roulette

For many traditional criticality applications, the use of importance sampling is not a real requirement because the property of interest is k-effective, an integral property of the system. The superhistory method employed in MONK [4] has an inherent pseudo importance sampling element to it by the means it employs to perform the source powering and this has proven to be successful in practical situations. However, for more specialised applications, the splitting and roulette option gives the user the capability to encourage the samples to concentrate on selected sections of the model by overlaying a map which gives the relative importance of sections of the model. This is particularly useful if the region of interest is in such a position that few samples would reach it. By overlaying a suitable importance map more samples can be encouraged to reach the required region thus giving a more accurate score. An example of the use of this method is in the analysis of small sample reactivity experiments whereby the splitting and roulette options can highlight the effect of the small sample introduction/removal.

The splitting and roulette method requires two additional sets of input: the first specifies a geometrical mesh and energy group structure in which the importance map will be used; the second comprises the importance map itself containing the importance of each mesh element in space and

energy. The ratio between the importance in adjacent meshes is used during the tracking process either to increase the number of samples but correspondingly reducing the weight of each (splitting when the weight increases), or to use a random number to determine if the sample should be removed (roulette when the weight decreases). The MONK method has been directly inherited from the shielding code MCBEND, where such techniques are routinely needed for ensuring the sampling concentrates on the important paths for a particular result (flux, dose etc.) that is not an integral property of the system. This inclusion has been facilitated as a direct result of the integrated Monte Carlo modular system from which versions of both MONK and MCBEND are assembled.

Enhanced Usability Options

The user of MONK has at his disposal a powerful calculation tool to help solve criticality analysis problems and in recent years this has been augmented by computers of such power that Monte Carlo calculations can be performed in minutes. To enable the analyst to make best use of this power, new code options have been developed to perform sequences of calculations in a planned and cost-effective manner. These developments have introduced the following improvements into MONK:

- MONK allows the user to parameterise the input data to facilitate the setting up of calculation sequences. The options here are:
 - basic parameterisation, where character strings are assigned to numerical values (e.g. @A=1, @density=1.234E-00)
 - formulae, where input strings can include algebraic expressions (e.g. SIN(30.0), @A+1.5)
 - calculation looping, repeated execution of the code following specified sequences of defined parameters (e.g. @RADIUS= 2.1; 2.2; 2.3)
 - multiple looping, where multiple parameter sequences can be varied in selected combinations
- To assist with using the sequence options above, MONK now allows the user to halt a particular MONK case if the value of k-effective is outside a pre-selected range. The option to halt as soon as possible those cases which are giving values of k-effective outside the acceptable range can be used to ensure that computing time is concentrated on the more important cases.
- MONK also allows the use of embedded files so that standard files can be accessed to include sections of input data

What Else?

Additional new facilities provided by or accompanying MONK8 include:

- Two new bodies are available for use in MONK8A: the hemisphere and the hexagonal prism, together with a new part type - the hexagonal array, which provides a means of tessellating the hexagonal prism. These options have been developed to extend the MONK modeller's armoury, particularly for waste management (hemisphere) and VVER fuel systems (prism).
- MONK8 is now available on the PC computer platform running Windows 95, 98 or NT
- The two-dimensional geometry visualisation productivity tool VISAGE (see Figure 3) and the three-dimensional visualisation tool VISTA-RAY (see Figure 4) have both been significantly enhanced (for example, the inclusion of dimension and material checking in VISAGE) and fully implemented on the PC platform.

- The MONK User Guide is now issued in paper and electronic format (Adobe Acrobat pdf format).
- The central MONK validation database continues to grow with the inclusion of many more experiments from the handbook from the International Criticality Safety Benchmark Evaluation Project (ICSBEP [5])

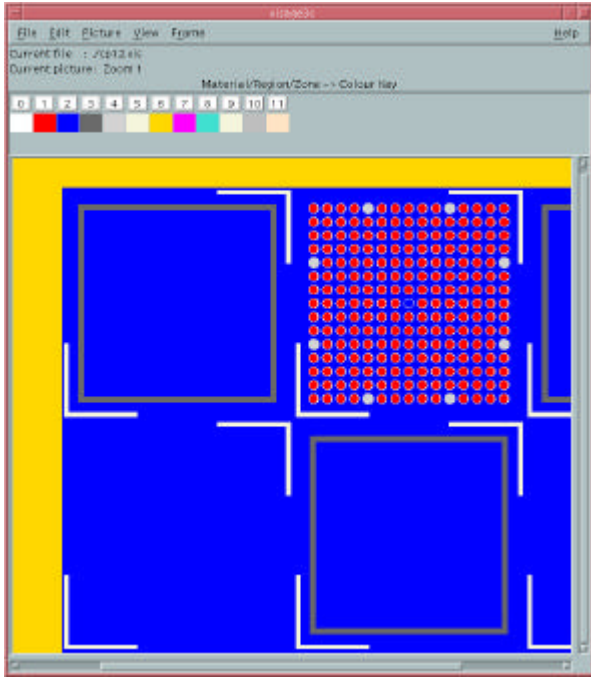


Figure 3 - VISAGE Image of Fuel Pool

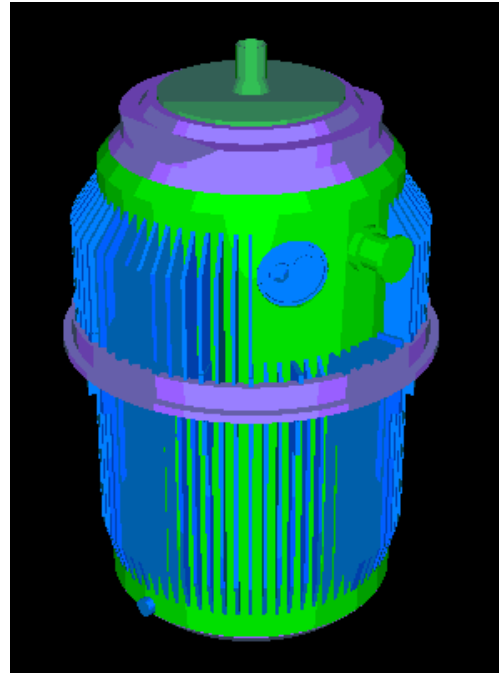


Figure 4 - VISTA-RAY Image of Cask

The Future

This paper has reviewed the outcome of the recently completed unification project - the code package MONK8. Several new features have been described, providing benefits to the new combined criticality and reactor physics MONK code users. This has been the latest part of an on-going MONK development schedule performed to ensure the code is best able to meet industry needs into the future. By working closely with major industry partners, the finished product has proven readily acceptable as a replacement for its two predecessor codes.

The development of MONK is now continuing in a variety of areas and significant active developments include:

- the production of an enhanced continuous energy collision package - this will provide improved physical modelling and even better data representation
- the development of a sensitivity option to help analysts assess the uncertainty in their calculations arising from nuclear data sources
- a component multiplication option to help assess interaction effects for multiple unit systems
- further geometry modelling developments to extend even further the MONK repertoire in keeping with code application needs
- more nuclear data choices, including the production of a JENDL-based library

- more supporting validation, drawing on the continued growth of the ICSBEP handbook

By means of this continuing response to customer needs, it is hoped that MONK can retain and further enhance its position within the criticality community.

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