The Development and Validation of a New Collision Processor for MONK

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This paper summarises the progress with a major development project for the MONK Monte Carlo criticality code, namely the development of a new collision processing modelling package and nuclear data library.

KEYWORDS: MONK, Codes, Software Development, Nuclear Data, Validation

1. Introduction

MONK [1)] is a well-established Monte Carlo code for the assessment of nuclear criticality safety problems, with over thirty-five years of successful application across the whole of the nuclear fuel cycle. Over the last decade, the development of MONK has been performed by a collaboration comprising British Nuclear Fuels plc (BNFL) and Serco Assurance, with the MONK code being distributed and maintained in use by Serco Assurance's ANSWERS Software Service.

Over the last few years, a substantial programme of regeneration and renewal has been in progress, to update and enhance various aspects of the MONK methods, data and software. The current production version of the code MONK8 [2)] was the culmination of one major strand of this programme, leading to the unification of two previously separate versions of the code (one for criticality, another for reactor physics). Another major strand, scheduled to appear in MONK9 next year, has been the development of a completely new neutron collision processing system and associated nuclear data library.

This paper outlines the historical development of the nuclear collision processing methods within MONK and the reasons for undertaking the present upgrading. It describes the structure of the new system and some of the important features of the methods used. Finally it summarises the results to date of on-going validation studies in which results obtained using the new collision processor have been compared with results from experiments or from other methods of calculation.

2. The Evolution of Collision Processing Methods and Data in MONK

2.1 The Development of DICE

For many years the nuclear collision processing has been handled within MONK by the DICE module, in conjunction with associated DICE nuclear data libraries. The DICE collision processor, the original version of which was developed at AWE Aldermaston in the 1960s, was incorporated into MONK more than twenty years ago following a development programme that enabled it to be used for general criticality applications. One improvement was to represent the cross-sections on a fixed hyperfine energy grid of 8220 groups. This provided a good representation of the resonance structure up to about 70 eV, and a subgroup method was incorporated to treat resonance shielding at higher energies.

Another development was to include modelling for the scattering of thermal neutrons by bound hydrogen atoms in water.

A pre-processing program called MOULD was used to generate the MONK nuclear data library from the basic data in the UK Nuclear Data Library (UKNDL), which was the only data source used by the code at that time. Data adjustments were made to improve agreement with critical experiments.

During the 1980's, when the UKNDL had been frozen and the Joint Evaluated File (JEF) was being developed, measures were adopted to accommodate data from JEF and other ENDF-format files within the DICE system. These included a new pre-processing route using the NJOY code. For these more modern nuclear data libraries, data adjustments were no longer required.

Further improvements have been made since then. The hyperfine energy grid has been revised to produce a scheme with 13193 groups, which provides improved modelling of resonance self shielding effects in the unresolved resonance range and a more accurate representation of cross-sections at thermal energies. Further enhancements have also been made to the modelling of thermal neutron scattering by bound atoms. DICE format nuclear data libraries derived from various sources (UKNDL, JEF2.2, ENDF/B-VI and JENDL3.2) are now available.

Validation evidence achieved by comparing MONK against experimental benchmarks supports the conclusion that with modern nuclear data libraries, the MONK code provides good agreement with measurement, generally within two standard

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deviations (combined calculation and experimental uncertainty), and often within one standard deviation. Given this current strong position, what were the driving forces for embarking on the major project of producing a new collision processing system for MONK?

2.2 The Need for a New Collision Processing System.

Although various factors contributed at the time, there were three main reasons that led to the initiation of this major programme of activity:

- An on-going objective of the BNFL/Serco Assurance collaboration is to strive for cost-effective improvements to the underlying physical realism available in MONK for both criticality and reactor physics applications. This objective can lead (and has led) to the provision of short-term user benefits in terms of new facilities to solve immediate issues, or to more strategic developments aimed at providing longer-term capability, confidence and security. With the passage of time, such developments in the collision processing area are made more difficult within the DICE system by the fact that it was designed originally for an evaluated data format that differed substantially from the modern ENDF format. Hence for the long-term, replacement rather than further enhancement was a clear requirement.
- Given its role, it is important that the MONK software can take advantage of modern developments in computer languages and systems and does not become frozen in time. Again with the passage of time this becomes increasingly difficult for the existing DICE system because its basic structure was designed for very early Fortran language versions and for computers with tape-based data storage and limited memory capacity. Again for the long-term, replacement rather than further enhancement was a clear requirement.
- Finally, and again looking to the long-term, both BNFL and Serco Assurance are committed to maintaining expertise in the Monte Carlo and nuclear data modelling areas. With personnel succession planning and sharing of expertise in mind, a major programme of activity provides a valuable framework to ensure expertise is passed on to the younger generation.

3. The BINGO Package

3.1 Structure

The new collision processing system for MONK has been named BINGO and consists of two parts: the pre-processor and the collision processor. The pre-processor is a program which is used to create a MONK nuclear data library by taking evaluated nuclear data files in ENDF-6 format and converting these data into a form suitable for Monte Carlo sampling. The collision processor is the module which forms part of the MONK code and which performs all the operations concerned with the modelling of neutron-nucleus collisions during the Monte Carlo process.

The components of the BINGO package are shown in Figure 1.

The pre-processor is a program which takes evaluated nuclear data files in ENDF-6 format and converts these data into the BINGO library format. Cross-section reconstruction and broadening are currently handled by NJOY, which is run as an external program. However, the GENEX code, originally written in the 1960's for use with UKNDL, is being re-written and will eventually be available to the pre-processor as an alternative to NJOY.

A BINGO nuclear data library consists of a collection of files, each one containing the data for a particular nuclide at a particular temperature. The data within each file are organised using a specially written database system.

The collision processor is a module within the MONK code. Its main functions are as follows:

- once the compositions of the materials present in the current case have been determined from the input, it reads the required data from the library and sets up pointers to enable items of data to be accessed quickly;
- during the tracking of neutrons, it is called to determine the mean free path of a neutron at its current energy in the current material, so that the code can sample for the position of the next collision;
- once a collision has occurred, it is called to determine the outcome of the event, such as the energy and direction of emergent neutrons.

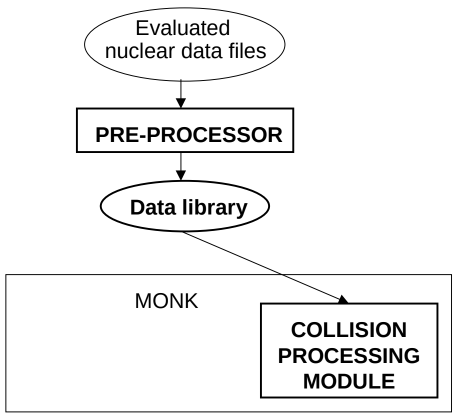

Fig.1 Components of the BINGO package

3.2 Methods

3.2.1 Cross-section Representation

Cross-sections are stored in the BINGO library as point values on an energy grid chosen so that intermediate values are adequately represented by linear interpolation. A different energy grid is used for each nuclide. This allows cross-section variations to be represented accurately in the resolved resonance regions for individual nuclides, while minimising the amount of data needed to represent smooth cross-sections. Numbers of energy points range from about 600 for hydrogen to 212000 for ^{238}U.

3.2.2 Unresolved Resonance Region

A subgroup method is used to treat resonance self shielding effects in the unresolved resonance region. It is a 2-subgroup technique, in which the cross-section in a narrow energy interval is represented as having two possible values. These values are calculated so that they produce the correct average cross-section in the interval when the nuclide is present at "infinite dilution" and at one other chosen dilution. The aim is to ensure that these cross-sections will also give an adequate representation of the resonance self shielding effect at intermediate dilutions. The two subgroup cross-sections are stored just like normal cross-sections over appropriate subdivisions of the interval, so that no special sampling procedure is required. This technique is similar to the one used in DICE, but is adapted for use with point-energy cross-sections and its accuracy has been improved by allowing the subgroups to be of unequal width.

3.2.3 Temperature Treatment

For any given nuclide, a BINGO library may contain cross-sections for a number of discrete temperatures. It is envisaged that, in practice, BINGO libraries will provide multi-temperature data for a set of the most important nuclides, while the data for the remaining nuclides will be for "room temperature" only. It is assumed that secondary energy and angle distributions are not dependent on the temperature, except at thermal energies. Thus the BINGO library files for elevated temperatures contain only the cross-section data (together with thermal scattering data in the case of bound atoms), and the code automatically refers to the room temperature file for the secondary distributions. At present, BINGO does not have the capability to interpolate between the temperatures given in the library. If the MONK user specifies an intermediate temperature, the code selects the data for the nearest available temperature.

3.2.4 Delayed Neutron Spectra

The BINGO library includes data for delayed neutrons from fission. These would enable the BINGO module to be used for kinetics calculations if required, but no such application is planned in the short term. Of more relevance for MONK is the fact that, even for statics calculations, the presence of the delayed neutron data allows the use of the correct spectra for delayed neutrons. For back compatibility, at present MONK is still using the prompt neutron spectrum for all fission neutrons, but it is planned to introduce the option to make use of the delayed neutron data in the BINGO library.

3.2.5 Thermal Neutron Scattering

For thermal neutron scattering by bound atoms, the data pre-processing is carried out by the BINGO pre-processor itself rather than by NJOY. This includes the processing of the $S(\alpha,\beta)$ data to calculate cross-section values and to generate the probability distributions to be used for sampling the α and β values from which the secondary energies and angles are calculated. The methods used in BINGO are, for the most part, similar to those used in the current version of DICE, but a number of improvements have been introduced. The main enhancement has been to introduce the modelling of coherent elastic scattering, which occurs in crystalline materials and which was not treated in DICE. It is important, in particular, for thermal neutron scattering in graphite.

As in DICE, thermal neutron scattering in most nuclides will be treated by a free gas model, but the aim is that BINGO libraries will include bound atom scattering data for a wider range of nuclides, to the extent that these are available in the evaluated nuclear data files.

3.3 Status

The BINGO module has been incorporated into a development version of the MONK code and this code version is now undergoing field testing in preparation for its formal release as MONK9.

The pre-processor has been used to generate a BINGO library from JEF2.2 data. This library contains data for 155 nuclides. Multiple-temperature data are provided for 35 of these nuclides. In general, a standard set of 23 temperatures from 293.6 K to 5000 K is used, but for nuclides with bound atom scattering data the set of temperatures for which $S(\alpha,\beta)$ data are given in the evaluated data file is used.

Further developments to BINGO will allow it to model photon production and photon and electron collisions, enabling it to be included in the general transport code, MCBEND. [3)]

4. Validation

4.1 General Plan

MONK has a large validation database comprising MONK models for experimental configurations, based mainly on specifications from the handbook of the International Criticality Safety Benchmark Evaluation Project (ICSBEP).[4)] At present the database contains over 80 experiments, and with most experiments including a number of separate variants of the geometry or materials, there are several hundred experimental configurations in total.

In order to obtain a full assessment of the accuracy of MONK using the JEF2.2-based BINGO library, calculations for the complete validation set are now in progress. However, in order to obtain an initial broad overview of the capabilities of the new system, a sub-set of calculations has been performed, with just one case chosen from each of the experiments. The calculated k-effective values could then be compared with the experimental values and with the results from MONK calculations already carried out using the JEF2.2-based DICE library.

In addition to the broad survey provided by calculations for cases from the validation database, a number of other comparisons are being carried out in more detail and to a higher precision. In particular, these include several benchmark problems that have been defined for international intercomparisons of criticality codes. Results for two of these are presented below; others are in progress.

Finally, a number of special studies are being undertaken to examine particular aspects of the nuclear data modelling in BINGO. One such study, described below, involves the calculation of the diffusion length for thermal neutrons in water.

The results of the calculations performed to date are included here for completeness but until the completion of the BINGO development programme and the release of MONK9, they should be regarded as provisional values only.

4.2 Cases from the Validation Database

MONK calculations using the new collision processor have been run for one case from each of the 85 experiments in the current MONK validation database using the data library generated from JEF2.2 data. The results have been compared with those obtained with the DICE collision processor using the JEF2.2-based DICE library. The cases in the database are divided into classes according to the physical form of the fissile material

- compound (e.g. oxide)
- solution
- metal

and according to the fissile element

- uranium
- plutonium
- mixed (U + Pu).

The results for these different classes are shown in Figures 2, 3 and 4. The deviation of the points from the diagonal line indicates the difference between the k-effective values obtained using BINGO and DICE, while the deviation from a k-effective value of 1.0 shows the difference between calculation and experiment.

In general, the differences between the calculations using BINGO and DICE are small and do not significantly alter the overall trends in the comparison with experiment, which are associated more with the basic evaluated nuclear data than with the representation of the data in the code. For example, it has been found that MONK with JEF2.2 data over-predicts the value of k-effective for plutonium solution systems by about 0.5%, and this can be seen in the results from the cases included in the present study, for which the mean k-effective value for plutonium solution systems is 1.0063 using DICE and 1.0056 using BINGO. Larger differences are observed for metal systems and a particular example is discussed in more detail below.

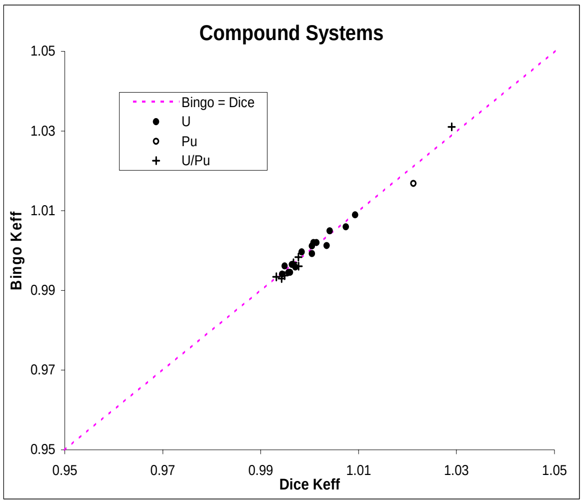

Fig.2 Results for Compound Systems

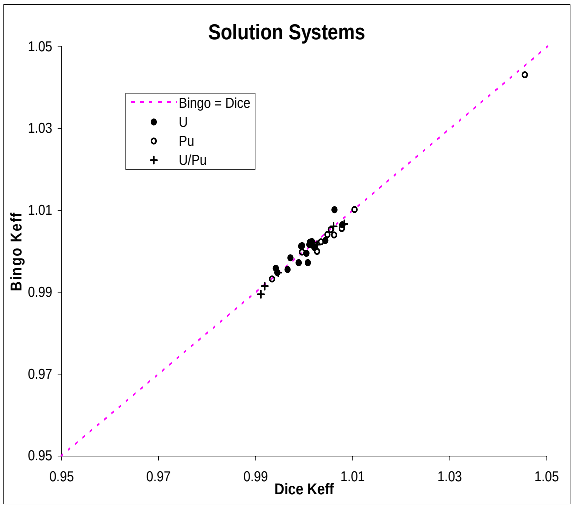

Fig.3 Results for Solution Systems

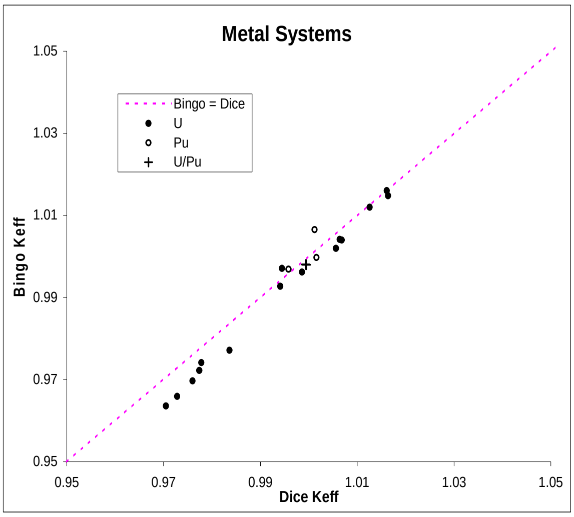

Fig.4 Results for Metal Systems

4.3 LWR Pin Cells

A number of simple light water reactor pin cell models have been defined for intercomparisons of different calculation methods using a common source of data, JEF2.2.[5] These benchmark models include cases with uranium oxide and mixed oxide fuel, and the effects of changes in temperature and water density are considered. Results from MONK (using the DICE collision processor) were included in this intercomparison, although its limited temperature modelling capabilities restricted it to the cases with all regions at 293 K. MONK with BINGO has now been applied to several of these pin cell cases, including those with elevated temperatures. Table 1 shows the k-infinity values obtained from MONK and from MCNP calculations performed by the University of Stuttgart as part of the intercomparison. The differences between the calculated k-infinity values are small, but the effects of the temperature changes calculated by MONK are slightly smaller than the effects calculated by MCNP.

Table 1 Results for LWR Pin Cells

Fuel type	Fuel temp. (K)	Water temp. (K)	k-infinity MONK BINGO	MONK DICE	MCNP
UOX	293	293	1.39015 ±0.00010	1.38910 ±0.00010	1.38994 ±0.00060
UOX	900	550	1.30860 ±0.00010	-	1.30678 ±0.00060
MOX	300	300	1.22607 ±0.00010	1.22600 ±0.00010	1.22700 ±0.00030
MOX	560	300	1.21338 ±0.00010	-	1.21270 ±0.00050

± numbers are Monte Carlo standard deviations

4.4 The GODIVA Experiment

The Los Alamos critical sphere experiments, GODIVA and JEZEBEL, were adopted as benchmark cases for an intercomparison of calculation methods using a common data source, JEF2.2.[6] For GODIVA, a sphere of highly enriched uranium metal, it was found that MONK with the standard DICE collision processor gave a k-effective value which, although closer to unity, was about 0.3% higher than the values given by a number of other codes. Investigations into the methods used in DICE showed that the discrepancy was caused mainly by some shortcomings in the method used to represent the dependence on incident neutron energy of the secondary energy distributions from fission and inelastic (continuum) scattering. Only by using a special version of the collision processor and data library, modified to remedy this deficiency, was it possible to obtain a consistent result. k-effective values obtained from these calculations and from new calculations using BINGO are presented in Table 2, together with the result from an MCNP calculation carried out by ECN, Petten, as part of the intercomparison. This shows that the improved methods used in BINGO have eliminated the previous discrepancy.

Table 2 Results for the GODIVA Experiment

Code	k-effective
MONK(BINGO)	0.9952 (±0.0001)
MONK(DICE - standard)	0.9985 (±0.0001)
MONK(DICE - modified)	0.9953 (±0.0001)
MCNP	0.9951 (±0.0001)

± numbers are Monte Carlo standard deviations

4.5 Thermal Neutron Diffusion Length in Water

One method of validating the treatment of thermal neutron scattering for bound hydrogen is to calculate the diffusion length for thermal neutrons in water and to compare this with measured values. MONK has been used to calculate the diffusion length by performing a fixed source calculation in one-dimensional plane geometry. An infinite plane source of thermal neutrons was modelled, with a thickness of water sufficient to allow the thermal neutron flux attenuation to settle down to its asymptotic form, $\exp(-x/L)$, where L is the diffusion length.

Results calculated with JEF2.2 data for three temperatures are shown in Table 3. These include the effect of the change in the water density. Measured values are also shown: the 20°C figure is a mean value derived by Butland from a survey of published measurements, while the values for 100°C and 250°C are measurements by Bowen and Scott.[7,8]

The results obtained using BINGO and DICE are very similar; this was expected since the methods used in DICE for hydrogen in water have been extensively upgraded over recent years and are largely unchanged in BINGO. The calculated diffusion lengths are about 3% lower than the measured values, but further studies will be needed to determine whether this is due to the methods used in the code or to the basic evaluated data.

Table 3 Thermal Diffusion Length in Water

Temperature (°C)	MONK BINGO	MONK DICE	Experiment
	Diffusion length (cm)		
20	2.670 ± 0.013	2.673 ± 0.004	2.75 ± 0.05
100	3.113 ± 0.010	-	3.186 ± 0.031
250	4.307 ± 0.015	4.295 ± 0.006	4.438 ± 0.044
	Calculation/Experiment		
20	0.971 ± 0.019	0.972 ± 0.018	
100	0.977 ± 0.010	-	
250	0.970 ± 0.011	0.968 ± 0.010	

± numbers include Monte Carlo standard deviations and experimental uncertainties

5. Conclusions

This paper has described the background, capability and results to-date for a major new development for the MONK code, namely the production of a replacement collision processor and nuclear data library. The development has now reached the final validation stage and further results will become available over the coming months in the period leading up to the release of MONK9. However, the results to date are very encouraging, and coupled with the additional benefits that have been and will be achieved by the code stakeholders, the MONK BINGO project looks set for a successful conclusion that will serve its user community well over the coming years.

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References

1) N. R. Smith, M. J. Armishaw and A. J. Cooper, "Current Status and Future Direction of the MONK Software Package", Proc. Int. Conf. on Nuclear Criticality Safety, ICNC2003, Tokai-mura, Japan, Oct. 20-24 (2003).
2) N. R. Smith, M. J. Armishaw, J. L. Hutton and J. Sidell, "The Unification of MONK - Extending the Monte Carlo Horizon", Proc. Int. Conf. on Nuclear Criticality Safety, ICNC1999, Versailles, France, Sep. 20-24 (1999).
3) G. A. Wright, E. Shuttleworth, M. J. Grimstone and A. J. Bird, "The Status of the General Radiation Transport Code MCBEND," Proceedings of an International Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications, Bologna, Italy, June 9-14 (2002).
4) OECD Nuclear Energy Agency, "International Handbook of Evaluated Criticality Safety Benchmark Experiments", NEA/NSC DOC(95)03 (2002).
5) J. L. Rowlands (editor), "LWR Pin Cell Benchmark Intercomparisons", OECD Nuclear Energy Agency, JEFF Report 15 (1999).
6) J. L. Rowlands (editor), "Intercomparison of Calculations for GODIVA and JEZEBEL", OECD Nuclear Energy Agency, JEFF Report 16 (1999).
7) A. T. D. Butland and C. T. Chudley, "Thermal Neutron Diffusion Data and the WIMS Scattering Models for Light Water", AEEW - R 701 (1970).
8) R. A. Bowen and M. C. Scott, Brit. Journ. Appl. Physics, Ser. 2, Vol. 2, 401 (1969).