THE ACCURATE DETERMINATION OF SUB-CRITICAL MARGINS TO MEET EMERGING CRITICALITY NEEDS

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ABSTRACT

This paper reviews recent and on-going developments associated with the MONK computer code aimed at enhancing the tools available to the criticality assessor. These developments are driven by the need to be able to accurately determine sub-critical margins for emerging challenges facing the criticality community, noting that the pursuit of increased accuracy is only appropriate if it is cost-effective. The paper reviews the developments under five main headings: Validation Database, Nuclear Data Library, Physics Modelling, Independent Capabilities and User Interface and concludes that with the strong applications-oriented input driving the development of MONK, the code is well-placed to meet its users' requirements well into the next century.

I. INTRODUCTION

Many contemporary criticality safety cases are based on a deterministic assessment of the safety of anticipated actual and hypothetical situations. Typically, this involves modelling a selection of arrangements in order to estimate the system multiplication for the worst-case scenario. Other factors allowing for the bias and uncertainty in the calculations also come into play, together with typically a fixed sub-critical allowance. This gives rise to the familiar inequality:

k-effective + other factors < sub-critical limit

This approach has served the industry well and has as principal attributes familiarity and simplicity of application. However, in the future, additional challenges will arise where it is felt this traditional approach will be difficult to sustain, including:

- Further requirements for economic savings (for example, fuel pool restrictions)
- Analysis of 'unknown' system compositions and geometry (waste handling)
- Incorporation of more realistic modelling (burn-up credit)
- The need to incorporate large time-scales (repositories)

This paper reviews the current activities that are being performed with respect to the Monte Carlo code MONK[1] to assist the criticality assessor in meeting these new challenges.

II. THE MONK SOFTWARE PACKAGE

MONK is a Monte Carlo neutronics computer code written to assist in the study of criticality safety problems. The origins of MONK can be traced to a code called GEM, which came out of the post-war nuclear weapons programme in the United Kingdom. A more recent major programme of development was stimulated by the expansion of the UK reprocessing industry and resulted in the production of MONK6 in the late 1980's. This has been followed by further enhancement and modernisation of the code and data, together with the development of supporting productivity tools.

The most recent version of the code is MONK7 and this is used throughout the UK nuclear industry wherever criticality problems arise, as well as in other countries. MONK is distributed and supported in use by AEA Technology as part of its ANSWERS Software Service, with the code development being managed by a collaboration comprising AEA and British Nuclear Fuels plc (BNFL). The strong links that exist between the user community and the code developers means that the development of MONK is focused and relevant to industry needs.

III. THE CHALLENGES AHEAD

In considering how criticality safety will be assessed to meet some of the new challenges, it seems likely that moves away from the traditional inequality approach will become more common as increasing use is made of probabilistic techniques, particularly for applications with large uncertainties on system composition and time-scales.

However it is also anticipated that the traditional deterministic inequality approach will remain in use with additional flexibility incorporated to meet some of the challenges identified above. This flexibility is expected to include the adoption of different limits (suitably justified) in different situations requiring more accurate identification and assessment of uncertainties. Changes in this area are already happening as due account of the full uncertainties associated with fuel irradiation are incorporated, and ways of systematically treating code/data bias effects are formulated.

To support the criticality assessor in meeting the challenges ahead, it is important that computer codes and data be developed with a clear focus on application requirements. Key development areas are:

- validation data - availability of a comprehensive code validation database which can be used to interpolate and extrapolate to meet changing needs
- nuclear data library - access to modern nuclear data evaluations and their optimal representation within code libraries to reduce biases
- physics modelling - the optimisation of methods approximations by physically realistic modelling
- independent capabilities - the availability of genuinely independent calculation methods to avoid the possibility of common-mode failure
- user interface - provision of supporting facilities to simplify code usage and reduce the scope for assessment errors

The close alliance between methods development and major application activities in the UK through the on-going collaboration between AEA Technology and BNFL is focused on providing solutions to the new challenges. The rest of this paper reviews the current activities that are being performed, with respect to the Monte Carlo code MONK, to assist the criticality assessor with the task of meeting the new challenges.

IV. PREPARING FOR THE FUTURE

A. Validation Database

For any modelling software package, it is essential for the user to be aware of both its accuracy and its range of applicability. For a code such as MONK, evidence of these is obtained mainly from comparisons of calculation with experiment, usually for critical systems. A large collection of such experiments has been analysed using MONK and this validation database underpins the use of the code in the majority of practical situations. Strict adherence to software version control and its distribution only in a licensed executable form mean that centrally performed validation results can be used directly by criticality analysts, thereby avoiding unnecessary duplication of effort. In the UK this approach is welcomed by the nuclear regulators as it provides confidence that the calculated results quoted in a safety case are robust and reproducible. For a commercial organisation using the code, further benefits therefore accrue as the approval process is expedited.

In the past there has been a tendency for data uncertainties to be ignored as they were small compared to the large pessimisms in the criticality safety analysis. However, these pessimisms are gradually being removed to meet the new challenges and so it is important that a full uncertainty assessment is performed, particularly as the relative lack of new experiments means that calculations will become even more important.

In criticality safety analysis at present, any limitations in the accuracy of MONK are normally incorporated into a revised estimate of the k-effective of the system by means of an error term (denoted here as E_{PD}) in the criticality safety inequality. Recent work suggests that this should be split into two components:

- E_{PD1} arising from the agreement observed between calculation and experiment
- E_{PD2} arising from the extrapolation required to move from experiment to intended application

In an ideal world, the criticality analyst would have at their disposal 'exact' experimental matches (in terms of nuclides, geometry and neutron spectrum) for the intended application. In this situation E_{PD2} would therefore be zero and the value of E_{PD} would depend solely on how the code results agreed with the experimental measurements.

In practice, relatively few exact matches exist although for the majority of current applications there is good supporting coverage. One of the benefits of the Monte Carlo method and the use of physically realistic interaction modelling in particular is the confidence with which interpolation (and limited extrapolation) of the validation data can be performed. However, gross extrapolation in the absence of experimental data should be treated with extreme caution.

To provide a solid foundation for the new challenges ahead, the MONK validation project is continuing to expand the central database, supported by traceable and independently reviewed records. Use is being made of the ICSBEP[2] data and the selection of experiments included in the database is customer-driven to meet emerging needs. Without such readily available validation data, significant cost penalties can be incurred by plant designers and operators.

Future needs include additional validation data for key fission product isotopes to support burnup credit and neutron poisons in both soluble and solid form. These are being addressed by use of extant experimental data and by the output from more recent experiments such as CERES[3].

Finally, the interpolation/extrapolation uncertainty (E_{PD2}) needs to be dealt with. Here, sensitivity analysis comes into play and the access to nuclear data uncertainty estimates and the means of utilising them is also being addressed. Covariance data have in the past been mainly of interest to nuclear data specialists but have the potential to fulfil a valuable role in supporting the criticality analyst in performing an assessment of uncertainties. Development of these data and the means of utilising them in a convenient form is another way in which the computer codes can become more powerful tools to assist the criticality assessor.

B. Nuclear Data Library

The accuracy achievable with MONK is ultimately governed by the accuracy of the nuclear data employed. The current version of the MONK nuclear data library is largely based on the tried and tested United Kingdom Nuclear Data Library (UKNDL). Notwithstanding the generally good agreement between MONK with its existing library and experiments, it was identified some years ago that a future requirement was to move to a position of employing libraries based on the international library JEF (Joint Evaluated File), to accrue the benefits of modern nuclear data evaluations, more widespread usage and international benchmarking and feedback.

The release of a frozen version of the JEF library (JEF2.2) by the OECD/NEA (Organisation for Economic Co-operation and Development/Nuclear Energy Agency) enabled code-specific libraries to be produced for benchmarking in the major application areas. In the UK, a JEF2.2-based MONK library has been assembled as part of a programme of work which has also included improvements in the resolution of U238 resonance region data and an optimised low energy cross-section data representation.

The MONK data library that has emerged from this work is the 1996 MONK library, derived solely from unadjusted JEF2.2 source data and utilising 13,193 energy groups (summarised in Table I). The more modern data and more detailed energy representation of the cross-sections means that for the majority of applications, the accuracy achievable using the unadjusted JEF-based library has been shown by validation studies to equal or surpass that achievable with the current standard UKNDL library (which includes some adjustments to key isotopes).

Upper Energy (eV)	No.of Groups	Group Range	Group Width (eV)	Comment
1.0060 E-5	1	1	6.039E-8	equal energy
0.1243034	603	2-604	0.015625	equal lethargy
0.1986363	60	605-664	0.0078125	equal lethargy
0.1992188	1	665	0.0005825	equal energy
3.0	1434	666-2099	0.001953125	equal energy
33.0	2560	2100-4659	0.01171875	equal energy
72.953125	2557	4660-7216	0.015625	equal energy
72.964327	1	7217	0.011202	equal energy
10.0150641E+3	5040	7218-12257	0.000976563	equal lethargy
14.8949554E+6	935	12258-13192	0.0078125	equal lethargy
15.0E+6	1	13193	0.1050446E+6	equal energy

Table I - Summary of Energy Group Scheme for JEF2.2-based MONK Library

Benchmarking of this new library has covered the same range of experimental systems as for the current standard library. It is currently envisaged that following the completion of on-going industry field trials, the new data library will be generally recommended and adopted. This will represent a major advance for the MONK package and ensure that its use into the future is directly linked to a modern data library and an active nuclear data evaluation project, in order to better meet increasing requirements for accuracy (where this is cost-effective) and uncertainty assessment.

C. Physics Modelling

In addition to the nuclear data library used by MONK, the other key determinant of the accuracy of the software is the neutron interaction modelling. In addition, more physically realistic modelling can make interpolation and extrapolation of the validation database more reliable (and more easily justifiable) as an aid to meeting new challenges.

The present combination of data representation and methods in MONK has been demonstrated by validation studies to provide a good model of the underlying physical processes. Users of MONK are very comfortable with using the existing package and have an acceptable knowledge of the uncertainties associated with the calculated results. However, the user community is interested in continuous improvement when this is cost effective and some requirements in this vein have been identified. Firstly, the basic collision treatment package in MONK was developed some time ago and targeted at different computer hardware than is used today. Secondly, there is some inflexibility built into the present system in terms of energy and temperature representation that needs to be overcome.

For these reasons, together with the continuing requirement for even more detailed and accurate computer calculations, a major programme of development is underway aimed at completely replacing the nuclear data pre-processing and interaction modelling part of MONK (and its sister shielding code MCBEND[4]). The aim is to significantly improve the modelling of current and emerging operational situations to reduce still further unnecessary approximations and the need for their justification.

The project is providing a new nuclear data and collision processing package for use by MONK and MCBEND to handle the collision of neutrons, gamma-rays and electrons/positrons, either individually or coupled. The software includes collision processing modules and a data pre-processing route for the preparation of evaluated nuclear data into libraries for use by the collision processor modules. To date, we have seen the completion of the data pre-processing component of the package with attention now directed to collision processing.

As a minimum requirement, the new package will model collisions sufficiently accurately that modelling errors are small compared to the uncertainties in the data. In addition, it is the intention that the package be sufficiently accurate not only to be of use in data benchmarking but also in the refinement of evaluated nuclear data libraries.

The principal modelling improvements of benefit to the criticality assessor are:

- Improved treatment of all secondary neutron laws
- Enhanced representation of cross-section by energy
- Even better representation of unresolved resonance data
- Incorporation of flexible temperature variations

It is considered that the emerging package will provide a further significant improvement in the physical realism of the MONK modelling and will aid criticality analysts in dealing with new problems.

D. Independent Capabilities

Much of the work described above is targeted at improving the accuracy of MONK by means of data and modelling, and improving the knowledge of that accuracy by means of validation. However, given the increasing reliance placed on calculation tools in criticality safety, it is important that they are not treated as infallible black-boxes.

MONK is a powerful tool in the hands of a knowledgeable and experienced assessor. The assessor uses judgement to decide which calculations are necessary and important and MONK has been developed to readily provide an accurate estimate of k-effective for the systems as modelled. However like all codes, MONK does not give any indication that the calculation requested is the ‘right’ one. It is therefore the combination of skilled intelligent user and powerful tool that creates the real force in criticality analysis as generally the most important question remains ‘have I done the right calculations?’. It is also the case that the role of the skilled assessor becomes even more important as traditional pessimisms are removed.

Numerous reports have been published and manuals written about the accuracy and features of computer codes. Indeed, today’s computer codes are of a power and sophistication only dreamed of in years gone by and we have the hardware and system software to make them very effective tools. The tendency though is to regard a calculated result as being ‘the answer’ and there is a trend to ignore weaknesses or limitations in applicability (or even a knowledge-gap in not recognising that such problems may exist).

One way to avoid over-reliance on one computer code is to retain the ability to utilise handbook data based on experimental measurements. Within BNFL a major programme of work is aimed at this, firstly by compiling existing handbook data in an easy-to-access electronic form. This provides handbook data on the screen of any analyst together with interactive access mechanisms to support code-based analysis.

The second part of this activity is to assemble a company-wide database of criticality knowledge based on design and operational analyses that have been performed. This is aimed at avoiding duplication of effort within the company in the future as well as trying to take maximum advantage from the wide range of extant criticality analyses performed within BNFL. For example, during the many years of analysis that took place on plants such as the Thermal Oxide Reprocessing Plant (THORP), a lot of data were produced for novel systems and in areas where the behaviour of the system was anomalous in terms of criticality safety. The current programme of work includes the identification, quality assurance and justification of novel data that could be useful in future assessments. These data are then added to the database with suitable caveats on the range of applicability.

Another way of avoiding reliance on any one code is to retain familiarity with another code, independently developed and maintained and preferably utilising a data library with some independence. Having two answers that agree does not mean the answer is right (two rights can make a wrong) but having two answers that differ significantly should be cause for investigation and possible concern.

Recognising that the data library/collision processing package is a key determinant of the difference between codes (assuming both have sufficiently powerful geometry modelling and source iteration capabilities), MONK has been developed to include a multigroup option utilising SCALE data libraries (see Figure 1). Thus the same system geometry can be modelled only once, yet calculations can be performed using both standard MONK hyperfine data and broad group SCALE data. This is proving to be a useful adjunct to the code and provides assistance to the assessor when performing interpolation or extrapolation of the validation database to meet new challenges.

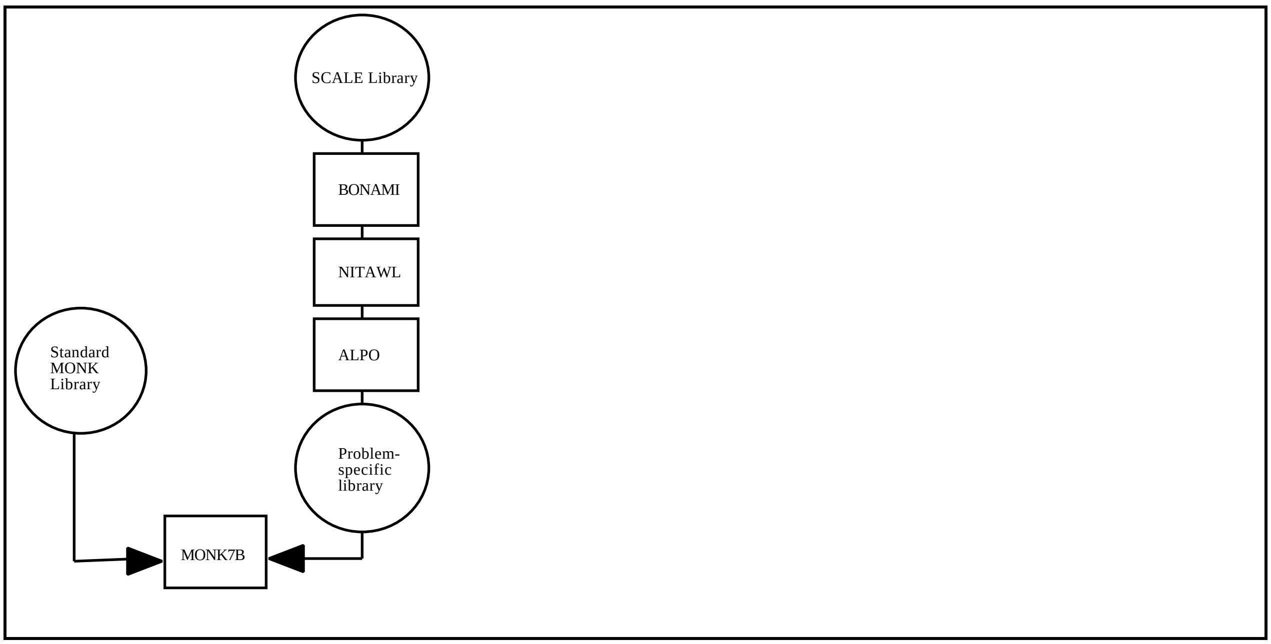

Figure 1 - SCALE data option for MONK7

E. User Interface

Over the last ten years the cost of utilising Monte Carlo software in real terms has plummeted due to the continually increasing power of computers. Today, a low-cost personal workstation can run MONK calculations faster than a mainframe serving a whole site at the time MONK6 first appeared. The real cost of assessment is now undoubtedly human cost and with increases in the power and sophistication of codes, it is important to make these increases available to the assessor in a convenient form.

The ease of using Monte Carlo codes for criticality analysis is governed largely by two components: the ease of preparing cross-sections for a given calculation and the ease of constructing a sufficiently accurate geometry model of the system under study. For MONK, the use of a problem-independent hyperfine library means that the cross-sections in the library can be used directly in a calculation, thereby simplifying the first component as far as is practicable. For geometry modelling, the MONK package is widely regarded as flexible and easy-to-use, something that is borne out on the regular training courses that are held.

Efforts at improving assessor productivity and accuracy have therefore been concentrated elsewhere and the following developments have been performed to ease the computer/user interface:

- Production of 2D and 3D visualisation tools (VISAGE and VISTA respectively) to comprehensively verify a MONK model.
- Production of the post-processing package VISTA-GRAPH, to tabulate, manipulate and view results (see Figure 2). This is aimed at improving the efficiency with which computed results can be utilised.
- Production of the post-processing package VISTA-TRACK, to display particle tracks superimposed on a view of the model. This can be used to increase knowledge of the system behaviour and confidence in the Monte Carlo sampling performed.
- Incorporation of post-processing sampling checks to review the accumulated Monte Carlo sampling activity and check for inconsistencies or inadequacies as an aid to increasing confidence.
- Addition of a user-extendible materials database to allow more easy specification of commonly needed compositions.
- Inclusion of a model library facility to provide the means of readily re-using defined and checked partial models in new calculations to avoid unnecessary duplication of effort and reduce scope for error
- Addition of parameter, formula and looping options to facilitate and simplify the specification of series of calculations, including the treatment of dependent variables.

All of these developments are available with the latest version of the MONK software package (version 7B) and are aimed at addressing key user interface issues associated with utilising sophisticated modelling tools to solve an increasingly diverse range of problems.

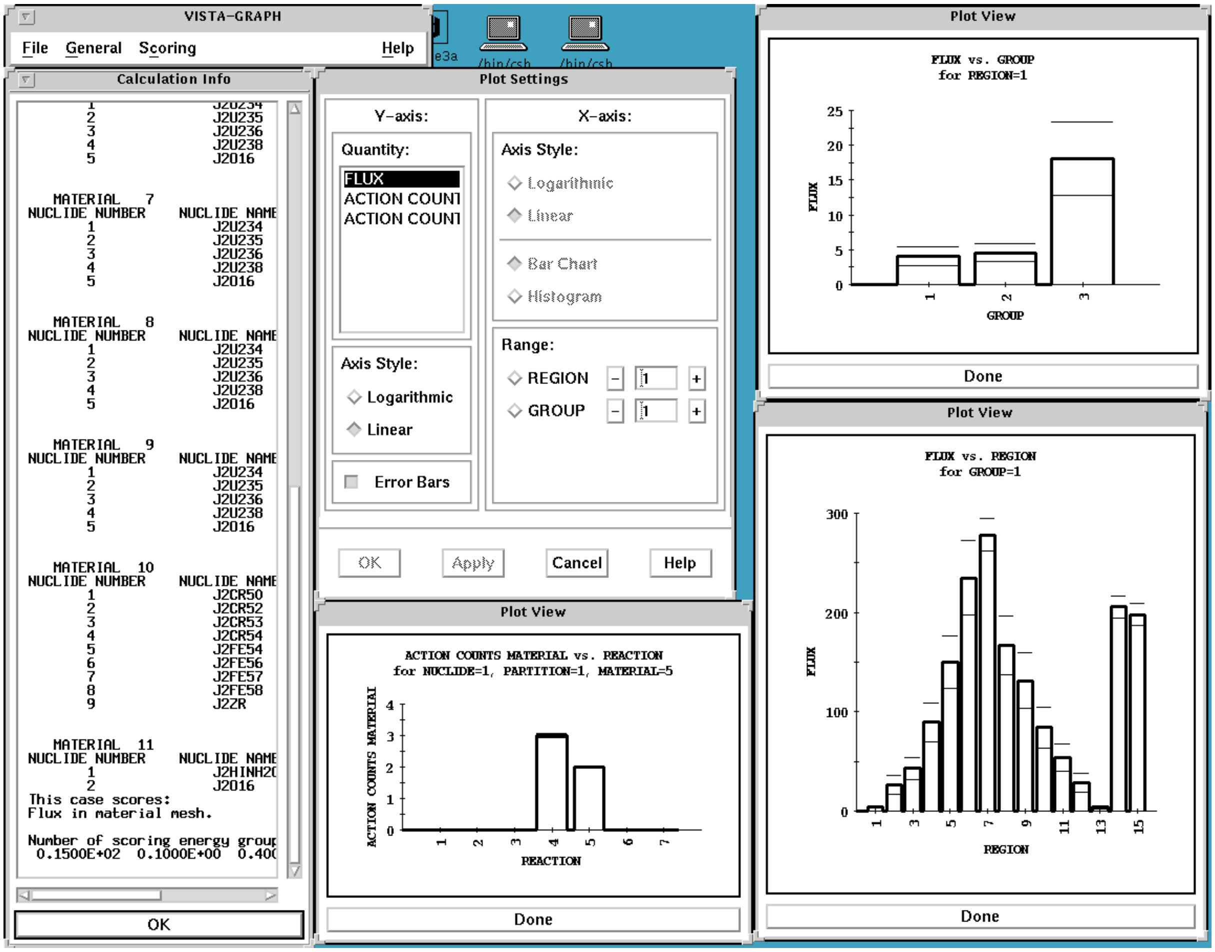

Figure 2 - Example of VISTA-GRAPH package

V. CONCLUSIONS

This paper has reviewed recent developments to the MONK computer code aimed at enhancing the tools available to the criticality assessor and the supporting knowledge-base underpinning its use. These developments have been driven by emerging challenges facing the criticality community and the need (when cost-effective) to be able to more accurately determine sub-critical margins. With the strong applications-oriented input driving its development, MONK is well-placed to meet its users' requirements well into the next century.

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