ANSWERS Conference Paper

Title:

SECURING THE MONK VALIDATION DATABASE

Authors:

Nigel R Smith, Jim Gulliford & David Hanlon
AEA Technology
Winfrith
Dorchester
Dorset, DT2 8DH
United Kingdom
44 1305 203260
44 1305 203030 - FAX
nigel.smith@aeat.co.uk

Peter R Thorne & Lyn M Farrington
British Nuclear Fuels plc
Risley
Warrington
Cheshire, WA3 6AT
United Kingdom
44 1925 832000
44 1925 833267- FAX

Date:

September 1995

Conference:

The Fifth International Conference on Nuclear Criticality Safety
Albuquerque, New Mexico, USA
17 - 21 September 1995

SECURING THE MONK VALIDATION DATABASE

Nigel R Smith, Jim Gulliford & David Hanlon
AEA Technology
Winfrith
Dorchester
Dorset, DT2 8DH
United Kingdom
44 1305 203260
44 1305 203030 - FAX
nigel.smith@aeat.co.uk

Peter R Thorne & Lyn M Farrington
British Nuclear Fuels plc
Risley
Warrington
Cheshire, WA3 6AT
United Kingdom
44 1925 832000
44 1925 833267- FAX

SUMMARY

For a criticality analyst to be able to judge the accuracy of the results from MONK calculations, the software package must be validated by comparison with suitable experimental data. More stringent regulatory requirements and an increasing emphasis on QA audit-trails have led to the initiation of a programme of work to expand the standard MONK validation database distributed as part of the code package. The main objective of this work is to secure a comprehensive centralised MONK validation database in a fully traceable form, in order to underpin the use of the code for the long-term future. This paper reviews the progress of the work to date.

INTRODUCTION

Software validation can be defined as the process of investigating whether the data, method of solution, code or calculational route is adequate for the solution of a particular problem. This may be achieved by comparison with experimental data and standard analytical solutions, or by comparison against another computer program. With particular reference to the Monte Carlo criticality code MONK7 [1], validation can be interpreted as the process of demonstrating that MONK can accurately reproduce experimental values of k-effective over a specified range of applications.

For a criticality analyst to have confidence in the results of MONK calculations for a particular type of system, and be able to judge how accurate these results might be, the software package (comprising the software itself and its nuclear data library) must be validated by comparison with suitable measured data. These data are normally provided by critical experiments. As far as practicable, the experimental configuration should have both neutron leakage and spectrum similar to that of the system being studied, as well as similarities in the materials and geometrical configuration. In addition, the experiment selected for the validation system should have quantifiable errors on the measured results that can be compared with the calculation uncertainty.

The MONK validation database comprises data from a wide range of experimental systems from a number of international laboratories. The validation database covers many of the materials and geometries that are encountered in the nuclear industry and is subject to on-going review and enhancement. However, more stringent regulatory requirements and an increasing emphasis on QA audit-trails have led to an acceleration of this enhancement activity, with a programme of work now on-going comprising the re-evaluation of key experiments and the analysis of additional experiments not previously studied.

This paper reviews the objectives and content of the MONK validation programme and summarises the results so far obtained. Further work that is proposed will also be described.

THE USE OF VALIDATION DATA

Validation of a software package such as MONK will normally be based on comparisons with experimental measurements. One important task for the criticality analyst is to identify validation data pertinent to his intended application in order to obtain the necessary confidence in the accuracy of his calculations. Clearly exact matches between experiment and application will be rare, but for many common requirements enveloping experiments can provide the level of confidence required. However given the decline in experimental programmes, a source of some concern must be that adequate experimental coverage for future applications will not necessarily exist.

The validation database for any software package has certain limits and it is important that the criticality analyst is aware of these. Should he encounter an application that extends beyond those for which validation data exists, it may be necessary to model additional experiments (should suitable ones exist) or use analytical techniques to estimate an adequate additional safety margin.

Three key attributes of the MONK software package make it particularly well-suited to the analysis of experimental data:

- the MONK geometry package allows experiments to be modelled in as much detail as necessary (provided that the experiments are well reported). This removes a potentially important source of uncertainty that may exist with other packages

- the use of a continuous energy nuclear data library and associated collision processing package offers a detailed representation of the collision mechanics that removes the inherent nuclear data pre-processing uncertainties of multi-group data

- the use of the superhistory powering algorithm means that systematic biases due to inadequate sampling and source normalisation can be effectively eliminated.

By performing software development and analysis within a fully implemented quality management system one can conclude that the major determinant for the accuracy of a MONK calculation is the quality of the basic nuclear data used to form its data library. However, it is important that due account of the experimental uncertainties be taken as well as those in the calculation when determining apparent code accuracy.

THE MONK VALIDATION DATABASE

MONK is distributed in ready-to-run executable form by the ANSWERS Software Service of AEA Technology. This is done to provide the level of quality assurance commensurate with the needs of safety analysis and for optimum user convenience. The route from source code to in-use executable code is maintained in a fully traceable form by ANSWERS for current and archived versions of the code. This removes a considerable QA burden from criticality analysts who are able to tie their use of the software directly to genuinely standard software versions which are rigorously controlled and uniquely identified.

Part of the MONK software package comprises a set of validation analyses, which due to the nature of software distribution can be used directly by safety analysts to support their applications. As the source code is not issued, the software version that safety analysts are using is identical to that used for the validation analyses as no local modifications are possible. This leads to a considerable cost saving in local installation, verification and QA.

The current validation programme for MONK comprises the re-analysis of selected key experiments and the study of additional experiments not previously analysed. In addition, greater depth is being added by the study of a range of configurations for each experiment, and estimates of the experimental uncertainties are derived by performing sensitivity analyses. This provides valuable additional information when trying to assess software accuracy.

The main objective of this work is to secure the MONK validation database in a fully traceable form, in order to underpin the use of the code for the long-term future. This is important for two reasons:

- the world-wide shortage of new experiments means that maximum advantage needs to be taken of the existing data; this becomes increasingly difficult with the passage of time

- major changes are envisaged in the MONK nuclear data area in the coming years with the development of a new neutron collision processing package and a nuclear data library based on JEF [2]; the availability of a comprehensive validation database is an essential part of being able to make that move.

To date the seventeen experimental programmes shown in Table I have been studied as part the new MONK validation programme and a further fifteen experimental analyses are currently in progress or planned for this year. Note that in each case several configurations involving different materials and/or geometries have been modelled so that the analyses listed in Table I total ~130 experiments. On-going analyses will increase this number significantly in the coming year, partly by drawing on the data emanating from the International Criticality Safety Benchmark Evaluation Project [3], which the MONK validation project is contributing towards.

It should be noted that the experiments described here are simply those that are currently included in the centralised MONK validation database distributed as part of the software package. Within the user community this set has been augmented by the study of additional systems of particular interest to the organisation in question. The aim of the continuing expansion of the centralised database is that the need for this additional work by the user community will diminish over the coming years as we encompass a broader and deeper range of experiments.

NUCLEAR DATA FOR CRITICALITY ANALYSIS

It was proposed earlier that the main determinant of the accuracy of a MONK calculation is the nuclear data. Most of the continuous energy nuclear data employed in MONK date from 1970's evaluations, although certain nuclides were updated by means of an adjustment programme during the 1980's. More recently we have seen the development of a

No.	Description	Laboratory
1.	UO_2 (2.35% enriched) pins in water with various absorbers	Hanford, USA
2.	UO_2 (4.75% enriched) pins in water (various pitches)	Valduc, France
3.	UO_2 (4.31% enriched) pins in water with various absorbers	Hanford, USA
4.	PuO_2/polystyrene compacts (11.46% Pu240)	Hanford, USA
5.	Plutonium nitrate solution spheres (4.6% Pu240)	Hanford, USA
6.	UO_2/PuO_2/polystyrene compacts (7.86% Pu)	Hanford, USA
7.	UO_2 (2.46% enriched) pins in water - close proximity storage	B&W, USA
8.	Uranium metal spheres (bare and reflected)	Los Alamos, USA
9.	Plutonium metal spheres (bare and reflected)	Los Alamos, USA
10.	Mixed nitrate solution cylinders (Pu/U = 0.3)	Aldermaston, UK
11.	Mixed oxide pins in water (20% Pu)	Hanford, USA
12.	Plutonium nitrate solution cylinders (43% Pu240)	Hanford, USA
13.	High enriched uranyl nitrate solution cylinders	Rocky Flats, USA
14.	Plutonium nitrate solution cylindrical annuli (19% Pu240)	Valduc, France
15.	Low enriched UO_2 powders	Springfields, UK
16.	Mixed oxide pins in water (20% Pu) with boral absorbers	Hanford, USA
17.	Mixed nitrate solution cylinders	Hanford, USA

Table I - Summary of New Standard MONK Validation Database as of April 1995 sophisticated thermalisation treatment for hydrogen in water and hydrogen in polythene based on more modern JEF data (in MONK7 [1]).

This work has resulted in a code that can compute the reactivity of the majority of systems of common current criticality interest to within about 1%. Clearly with future requirements to study new areas such as the MOX fuel cycle and burn-up credit, further validation of the nuclear data is required and this will almost certainly mean that additional high-quality critical experiments will be needed. Industry is demanding calculational accuracies which are approaching the existing precision of the nuclear data and is keen to avoid economical penalties incurred by the adoption of restrictive operating limits to overcome inadequacies of the nuclear data and its representation in application codes.

On the nuclear data front progress is continuing, with a MONK library based on JEF2.2 currently being benchmarked [2]; current indications are that this development will provide a useful improvement to the accuracy of MONK. JEF is an international file of nuclear data which in recent years has seen close collaboration with the USA work on ENDF. In addition, to complement the advances being made in nuclear data evaluation, a major programme of software development is now underway to produce a new generation collision processing package for MONK and the general Monte Carlo particle transport code MCBEND [4], which will become available for general use in the next two years. The on-going validation programme described in this paper will contribute to the process of bringing this new work into general use by evaluating predictive accuracy.

RESULTS OF MONK VALIDATION ANALYSES

Turning back to the present, this section summarises the results of a selection of the experimental evaluations already performed and identifies areas where it is to be anticipated that improvements to the accuracy of the code will occur.

The experiments that have been evaluated have been studied within a fully developed quality management system which has involved standard software usage, detailed geometry checking using the high-resolution graphical tool VISAGE [1] and independent checking and review by criticality analysis, experimental operations and code applications specialists.

Uranium Lattices

A large number of configurations have been studied in this area comprising the four experiments in the validation database summarised in Table I (experiments 1,2,3 and 7) together with a DIMPLE reactor experiment which has not yet been formally added to the validation database (this has been included to provide some laboratory independence at the under-moderated end of the range). The results for these cases are summarised in Table II (with one standard deviation uncertainties in brackets).

Exp. No.	No. of cases	Experimental Result	Mean MONK k-effective
1	9	1.0000 (0.0020)	1.0036 (0.0003)
2	9	1.0000 (0.0040)	1.0089 (0.0018)
3	8	1.0000 (0.0017)	1.0026 (0.0005)
7	8	1.0000 (0.0020)	1.0050 (0.0039)
DIMPLE S03	1	1.0000 (0.0020)	1.0100 (0.0010)

Table II - Results for Uranium Lattices

The results show that for low-enriched uranium lattices MONK tends to over-predict k-effective by between 0.3 and 1.0%. The results are plotted in Figure 1 against H:U (fissile) and this figure suggests that there may be a tendency towards increasing over-prediction with reducing moderation level. Comparison with sub-critical measurements performed in the DIMPLE reactor support this general conclusion. However in general the results for these systems show good agreement with experiment, in most cases close to the two standard deviation experimental uncertainty.

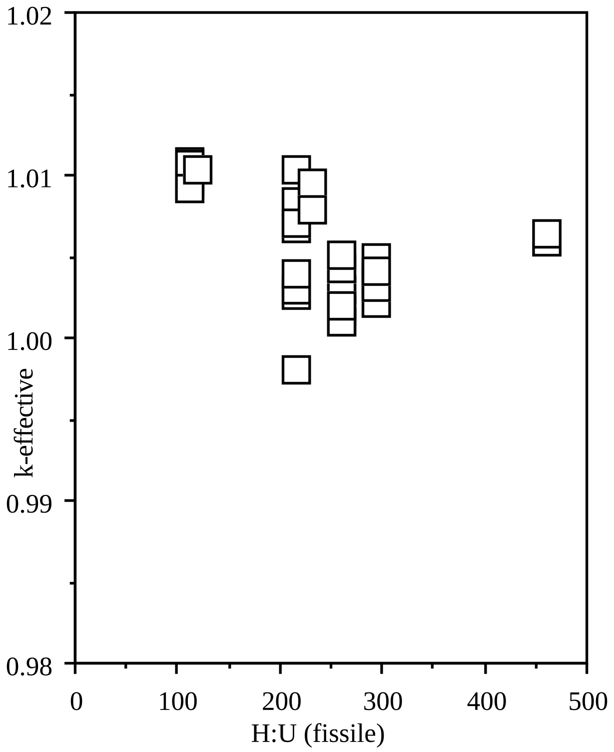

Figure 1 - Calculated k-effective against H:U for Low-enriched Uranium Lattice Experiments

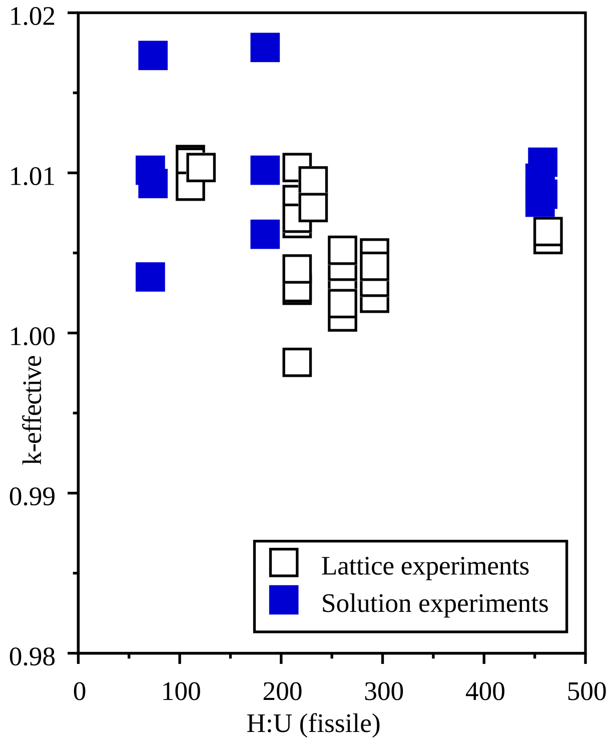

Figure 2 - Calculated k-effective against H:U for Uranium Lattice and Solution Experiments

If we include the solution experiment (no.13 in Table I) the change in agreement with H:U is not so clear with little variation in over-prediction between the solution concentrations, although the estimated experimental uncertainty is somewhat larger for the solution experiments. The results including the solution experiment are shown in Figure 2.

Mixed Oxide Lattices

In this category at present two experiments have been evaluated, both from the Hanford Pacific Northwest Laboratories involving fuel rods containing ~20% Pu. The results for these cases are summarised in Table III.

Exp. No.	No. of cases	Experimental Result	Mean MONK k-effective
11	4	1.0000 (0.0030)	0.9902 (0.0025)
16	8	1.0000 (0.0025)	0.9896 (0.0029)

Table III - Results for Mixed Oxide Lattices

These results provide evidence of an under-prediction for such systems of the order of 1%, although as these experiments were performed at the same laboratory using the same fuel rods some laboratory independence is desirable to support this conclusion. This is being addressed in the current programme.

Mixed Nitrate Solutions

Two experiments have been studied to date in this category, one from Aldermaston and the other from Hanford. In each case the plutonium made up about 30% of the total plutonium plus uranium, with the uranium being natural. The results are shown in Table IV.

Exp. No.	No. of cases	Experimental Result	Mean MONK k-effective
10	10	1.0000 (0.0025)	1.0058 (0.0043)
17	13	1.0000 (0.0035)	0.9954 (0.0041)

Table IV - Results for Mixed Nitrate Solutions

There is a significant difference between the two sets of calculated results, despite the similarities of the solutions (and geometries, as both experiments comprised single cylinders reflected by water). The difference is more apparent if the results are plotted by moderation level (H:Pu is used as plutonium is the principle fissile isotope). Figure 3 shows that this indicates a difference of ~2% at the low end of the H:Pu, well outside the estimated experimental uncertainty.

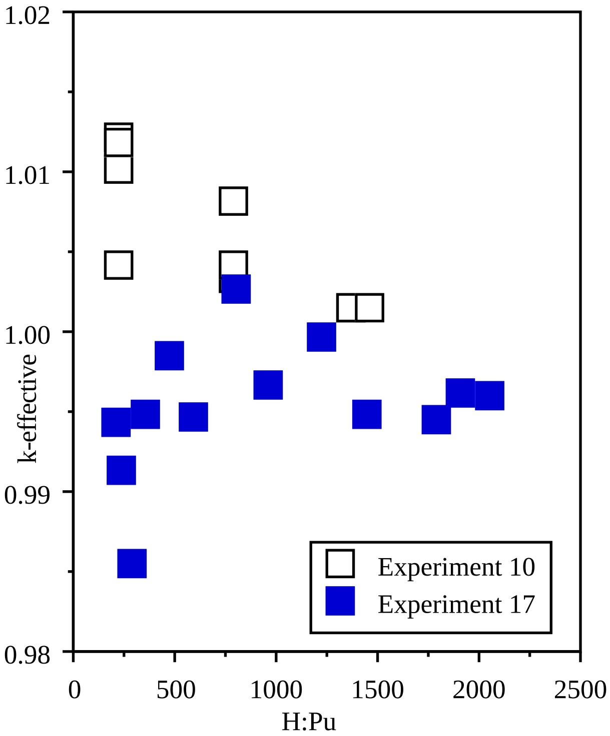

Figure 3 - Calculated k-effective against H:Pu for Mixed Nitrate Solution Experiments

If we calculate an equivalent H:Pu ratio for the mixed oxide lattice experiments described above, we can see that where the moderation ranges overlap the mixed oxide cases agree well with experiment 17 (see Figure 4). This leads us to question the reliability of experiment 10 and further experiments are now being studied to resolve this issue.

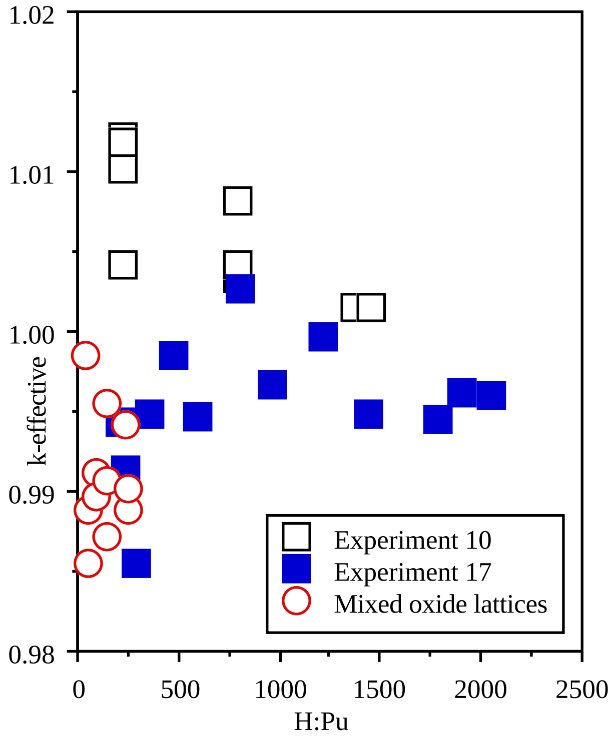

Figure 4 - Calculated k-effective against H:Pu for Mixed Nitrate Solution and Mixed Oxide Experiments

Plutonium Nitrate Solutions

The standard MONK validation database contains three plutonium nitrate solution experiments, two from Hanford and one from Valduc. These have been augmented by the results from six experiments from the ICSBEP [3]. The results obtained are summarised in Table V (note that PU-001 in the table is short for PU-SOL-THERM-001, the reference used in [3]).

If we plot these results against H:Pu we see a very consistent accurate prediction over the whole moderation range (see Figure 5).

Exp. No.	No. of cases	Experimental Result	Mean MONK k-effective
5	12	1.0000 (0.0021)	1.0040 (0.0077)
12	9	1.0000 (0.0020)	1.0034 (0.0012)
14	8	1.0000 (0.0027)	0.9984 (0.0013)
PU-001	6	1.0000 (0.0050)	1.0038 (0.0036)
PU-002	7	1.0000 (0.0050)	1.0032 (0.0013)
PU-003	6	1.0000 (0.0050)	1.0009 (0.0034)
PU-004	13	1.0000 (0.0050)	0.9972 (0.0030)
PU-005	9	1.0000 (0.0050)	0.9999 (0.0023)
PU-006	3	1.0000 (0.0050)	0.9983 (0.0003)

Table V - Results for Plutonium Nitrate Solutions

By including the mixed cases on the same graph (see Figure 6), we still see reasonably consistent prediction. However the spread of results is now larger than would be expected based on the estimated experimental uncertainty, particularly at the low H:Pu end of the range. This could mean that the experimental uncertainty has been under-estimated or that there are additional problems or uncertainties in performing solution experiments that have not been taken into account. Care must therefore be taken when using solution experiments to support code applications as the uncertainty on the conclusions could be quite large. Due account needs to be taken of this when performing criticality assessments. For our part we propose to study more experiments and perform statistical analysis of the results to try to come to more definitive conclusions.

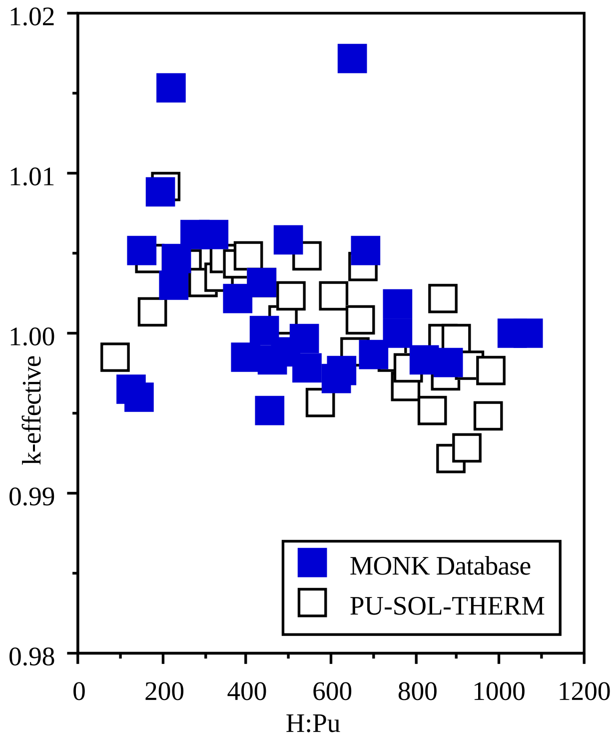

Figure 5 - Calculated k-effective against H:Pu for Plutonium Nitrate Solution Experiments

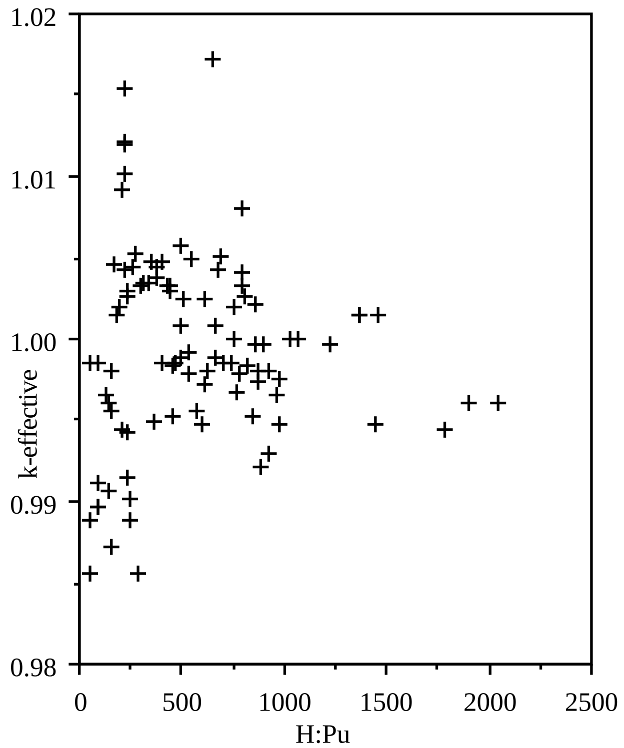

Figure 6 - Calculated k-effective against H:Pu for Nitrate Solution and Mixed Oxide Experiments

CONCLUSIONS

This paper has reported on a programme of work aimed at securing a comprehensive centralised validation database for the MONK software package. A number of experimental evaluations have already been performed and many more are now either in progress or planned. The work performed to date has demonstrated that MONK computes the system multiplication for the majority of experiments to within 1%, and in many cases significantly better. The results for selected key categories of systems studied so far lead to the following conclusions about MONK7 in conjunction with its UKNDL-based nuclear data library:

- For low-enriched uranium lattice systems, MONK calculates the experimental multiplication factor close to the level of the experimental uncertainties. For a set of over thirty experiments from five experimental programmes, the MONK calculated results over-predict the experimental values by an average of about 0.5%. These results demonstrate than MONK can be used with confidence for the majority of LWR fuel operations.

- For the mixed oxide lattice systems studied to date, MONK under-predicts the experimental multiplication by up to 1%. However these experiments are not particularly representative of LWR re-cycle operations and so further experiments are now being studied to provide additional supporting validation data. These additional experiments will also provide some laboratory independence.

- For plutonium and mixed nitrate solutions MONK predicts the experimental multiplication accurately, in most cases within the experimental uncertainties. It should be noted though that as a set, the spread of calculated results is larger than would be expected from the estimated experimental uncertainties. This suggests that there may be additional inherent uncertainties associated with solution experiments and due note of this spread needs to be taken when utilising validation data for such systems. However as a predictive tool, MONK again performs well in comparison with experimental data.

In addition to extending the validation database further, work is also in progress aimed at improving the continuous energy collision modelling of MONK and over-hauling the nuclear data library by the provision of a new library based on JEF evaluations. The validation programme described here will enable a widespread evaluation of such major changes to be performed before releasing a new version of the MONK software package to the nuclear industry. In the meantime, the results described in this paper indicate that MONK can be utilised with confidence for criticality safety analysis over a wide range of systems of interest.

REFERENCES

1 Smith N R and Morrell G A, "An Introduction to MONK7", *International Conference on Nuclear Criticality Safety ICNC'95* (Albuquerque, 1995)

2 Gulliford N T, Hanlon D and Smith N R, "Application of JEF Data for Criticality Calculations", *International Conference on Nuclear Criticality Safety ICNC'95* (Albuquerque, 1995)

3 Briggs J B, "The International Criticality Safety Benchmark Evaluation Project", *International Conference on Nuclear Criticality Safety ICNC'95* (Albuquerque, 1995)

4 Chucas S J, Curl I J, Shuttleworth E and Morrell G, "Preparing the Monte Carlo Code MCBEND for the 21st Century', *8th International Conference on Radiation Shielding* (Arlington, 1994)