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Summary

The JEF library is the identified future source of nuclear data for use in the UK. The release of a frozen version of the library during 1992 (JEF2.2) enables code-specific libraries to be produced for evaluation in the major application areas. Performance feedback from these evaluation studies can then be provided to the evaluators.

One of these application areas is criticality safety where the standard UK calculational tool is the Monte Carlo computer code MONK. MONK contains a continuous energy representation of the neutron collision processes, enabling fine detail and good physical realism to be employed.

Work leading to the production of a MONK library has been performed during 1992/93. This report describes the use of this library to evaluate the performance of the JEF2.2 library for a number of key critical experiments.

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1. INTRODUCTION

Criticality safety is a major consideration in operations associated the the production, transportation, storage and reprocessing of nuclear reactor fuel. Modern nuclear criticality safety analysis places great reliance on calculations performed using computer codes, in particular those employing the Monte Carlo method of solution. In the United Kingdom the acknowledged standard Monte Carlo code for criticality safety assessment is MONK [1].

MONK is a Monte Carlo neutronics computer code developed for use in the study of criticality safety problems. The principal aim of MONK is to calculate the effective neutron multiplication factor for arrangements of nuclear materials by computer simulation of the behaviour of a sample of neutrons. The actual number of samples followed determines the statistical precision of the final scored parameters which include a minimum variance estimate of k-effective, neutron fluxes, neutron currents and reaction rates.

The full geometry modelling potential of the Monte Carlo method is exploited in MONK. The code's geometry modelling package consists of two complementary components. The first is a set of generally orientated simple bodies which can be used in any combination to define the major component outlines. This is augmented by a collection of special options called hole geometries based on an elegant algorithm known as Woodcock tracking. It is these hole geometries that provide a lot of the more complicated fine geometrical detail, as well as offering a short-cut to the specification of some of the more commonly occurring configurations. The two components in combination provide a geometry modelling package of unrivalled power and flexibility.

MONK estimates the system multiplication factor k-effective using a staged calculation, where each stage consists of a fixed number of neutron superhistories. A neutron superhistory is the set of tracks followed by a neutron and its entire fission progeny through a fixed maximum number of fission generations (normally 10). By this means a stable calculation of the scored values of k-effective and its variance is achieved which is essentially free from statistical sampling bias.

MONK can access a wide range of nuclear data libraries which means that extensive cross-checking is possible for unusual situations. The standard MONK nuclear data library is an ultra-fine compilation employing 8220 energy groups over the range 0 to 15 MeV. This library is used in conjunction with a continuous energy collision processing package, providing a very detailed and accurate physical modelling capability. Due to this detailed representation no resonance correction treatment is required and the library can be employed directly by MONK. This means that the need for pre-processing codes and their inherent problems and limitations is eliminated.

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 now-defunct United Kingdom Nuclear Data Library (UKNDL). An identified future requirement is to move to a position of employing libraries based on the European library JEF, so that advantage can be taken of modern nuclear data evaluation work.

The release of a frozen version of the JEF library during 1992 (JEF2.2) has enabled code-specific libraries to be produced for evaluation in the major application areas. Feedback on the performance of the new libraries in these evaluation studies can then be provided to the evaluators. Work leading to the production of a JEF2.2-based MONK library has been performed during 1992/93 and this library has been employed to evaluate its performance in calculating the system multiplication of a number of important international critical experiments.

This report is concerned with the application of MONK to the modelling of critical experiments from five international programmes. The results of MONK calculations using the JEF2.2-based nuclear data library are reported and compared with experimental measurements and results obtained with the currently employed UKNDL-based library.

2. PREPARATIONS FOR USING THE JEF-BASED LIBRARY

Before calculations using the JEF-based library could be performed, some enhancement of the standard version of the MONK code was required in order to access the latest thermal scattering data. The treatment of thermal neutron scattering is an important part of a Monte Carlo particle transport computer code. This is particularly so for criticality applications where the system multiplication, k-effective, can be significantly affected by the calculated thermal flux spectrum.

The current production version of the MONK criticality code is identified as MONK6B. MONK6B contains a thermal scattering collision package which employs a free gas model for all nuclides with the exception of hydrogen when bound in water, which is normally the most significant thermal scattering effect of interest in the area of criticality safety assessment. The bound hydrogen model is a simplified model embodying a number of adjusted parameters and provides adequate accuracy for the majority of common criticality application requirements. However some limitations can be identified:

- the model treats hydrogen at only one temperature (293K) and a significant amount of work would be required to overcome this restriction
- no treatment exists for hydrogen bound in other materials, although the nuclear data does exist
- the model is not able to respond easily to updates in the nuclear data

These deficiencies can be overcome by sampling from the thermal scattering models used by the nuclear data library and employing the data contained therein. The JEF nuclear data library describes thermal scattering in terms of two models, inelastic and elastic scattering; the latter is sub-divided into incoherent and coherent forms, depending on the structure of the medium. Scattering by hydrogen in water is unusual in that it is adequately modelled by inelastic scattering only, whereas nuclides in most other situations also exhibit one of the two forms of elastic scattering.

A new thermal scattering package has been produced for the MONK code which overcomes the above limitiations [2]. This package will be part of the the next generation MONK code (MONK7) which is currently being developed. However at this stage the new generation code is not in a suitable state for use in a nuclear data benchmark exercise. Therefore in order to adequately benchmark the JEF2-based library in MONK it has been necessary to produce a special development version of MONK6 so that the JEF thermal scattering data can be employed in the experimental analyses.

The initial stage of this project therefore consisted of installing the new thermal scattering collision package in a special version of MONK6 for use in the JEF benchmarking process. This version is identified in this report as MONKDEV. This installation stage comprised extracting the new thermal scattering collision package from the MONK7 development environment and including it within an otherwise standard version of MONK6. Due to radical changes that have recently been made to the software development environment for the main UK Monte Carlo particle transport codes, this process was far from straightforward. In addition as the new thermal scattering collision package was part of a developing code and had yet to receive full testing, some problems were encountered during the testing of the MONKDEV code. These were resolved as part of this project before the benchmark exercise commenced.

Following the completion of this preliminary testing phase, further problems were encountered with the processed JEF2.2 data for certain nuclides. Significant effort was expended as part of

this project investigating these problems with the result that minor modifications to the latter stages of the JEF2.2 to MONK processing route were required. Once these were made no further significant problems were encountered.

The production of the development version of MONK enables direct comparisons to be made with results obtained using the current production code MONK6B. This inter-code comparison (essentially an inter-library comparison of JEF2.2 and UKNDL data) forms part of this report.

Note that the JEF2.2/MONKDEV combination is not a recognised issued version of MONK6 and the results obtained from it are in no way indicative of the accuracy obtained with the current production version MONK6B. It should also be noted that this report considers only a limited sub-set of the range of applications for which MONK6B is employed.

3. ANALYSIS OF BENCHMARK EXPERIMENTS

With the increasing reliance on computer calculations the question of computer code validation becomes ever more important. For a code such as MONK validation can be defined as ensuring that a version of MONK can calculate the system multiplication factor adequately for an appropriate range of well characterised experimental configurations of fissile material.

In order to provide a fully documented route from experimental measurements to calculational analysis, a modern QA procedure has been produced for the analysis of benchmark experiments. This procedure has been employed for the experiments analysed in this report and is summarised below:

(1) Locate experimental description documents and any other supporting references, such as experimental programme summaries or other code analyses. Confirm that the data presented are consistent and adequate for complete and accurate MONK models to be created.

(2) Extract and record all relevant data from the experimental documentation. Any approximations or assumptions must be fully justified by rigorous argument or by supporting calculations.

(3) Create MONK models based on the extracted data using currently recommended code options. The derivation of all code input data items not explicitly given in the experimental documentation must be recorded.

(4) Perform detailed checks on the problem geometry using the VISAGE package [1].

(5) Obtain a check of the MONK input specifications by an independent code user.

(6) Perform MONK calculations using an official ANSWERS version of the code.

(7) Examine the output from the calculations, record the relevant results and identify the checks that have been performed to determine the adequacy of the calculations.

(8) Perform a sensitivity study in order to estimate the total experimental uncertainty.

(9) Prepare a validation report which describes the MONK models and records and discusses the results of the calculations.

(10) Obtain a peer review of the validation report by a representative from each of the following fields: experimental analysis; criticality analysis; and mathematical modelling.

Note that for the calculations employing the JEF2-based library the code used at step (6) is not an official ANSWERS version of the code but a special development version as noted in Section 2.

4. SELECTION OF EXPERIMENTS

The existing validation database for MONK is wide ranging and is designed to provide some base level of support for the use of the code across the entire nuclear fuel cycle. Experiments in the database have been chosen from a range of international laboratory programmes performed over the past thirty years or so. For this report it has only been possible to perform calculations covering a more limited range and so it was decided to concentrate a significant amount of the effort on one application area. The application area chosen was low enriched uranium reactor fuel transportation and storage and three experiments of relevance were chosen. However in order to get some information on the performance of the JEF plutonium data, two further experiments were chosen from the fuel processing application area. The full list of selected experimental programmes is:

1 arrays of 2.35% enriched UO_2 pins in water with various fixed absorbers [3]

2 array of 4.75% UO_2 pins in water with various levels of moderation [4]

3 arrays of 4.31% UO_2 pins in water with various fixed absorbers [5]

4 PuO_2/polystyrene compacts (11.5% Pu240, H:Pu ratio = 5) with Plexiglas reflector [6]

5 PuO_2/UO_2/polystyrene compacts (7.86% Pu, H:(U+Pu) ratio = 52) with Plexiglas reflector [7]

To provide the required level of QA and accuracy necessary, detailed re-evaluations of the selected experiments have been performed. This enables calculation bias to be sensibly compared with quantified experimental uncertainties. In each case a number of configurations have been chosen from the experimental programme in order to assist with the uncertainty analysis. The description of the analysis of the experiments is given in Section 5 which is split into five sub-sections, one for each experiment.

5. EXPERIMENTAL ANALYSES

5.1 Experiment Number 1

5.1.1 Experimental Description

The experimental programme from which the experiments were selected was performed at the Battelle PNL Critical Mass Laboratory [3], and was completed in 1976, with funding from the US Nuclear Regulatory Commission.

The experimental programme considered water moderated and reflected clusters of low-enriched UO_2 fuel rods, both with and without interspersed neutron absorbing materials in the form of plates. The aim of the programme was to provide data for validating methods of calculation and nuclear data used in criticality assessments of LWR-type fuel element transport packages and similar systems.

The experimental configuration comprised three clusters of LWR-type fuel rods within a large tank containing water. In most of the experiments a neutron-absorbing plate was located between the central cluster and each of the other two clusters. For a given cluster size, the separation distance between the clusters (X), and when present, the separation distance between the central cluster and the absorbing plates (G), acted as the experimental control mechanisms in the approach to critical.

Figures 5.1.1 and 5.1.2 give an overall view of the experimental configuration. Figure 5.1.3 gives an enlarged view of the central cluster, and shows more clearly the separation distances X and G. Note that the system is symmetrical with respect to the separation distances, and that the distances are measured to the edge of a notional fuel cell boundary.

The following range of neutron absorbing plates was employed in the experimental programme:

- 304 L Steel with 0.0, 1.05 and 1.62 wt% Boron
- Boral
- Copper with 0.0 and 0.99 wt% Cadmium
- Cadmium
- Aluminium
- Zircaloy-4

In addition some experiments were performed without the neutron absorbing plates.

The fuel used in all the experiments was aluminium-clad 2.35 Wt% U235 enriched UO_2 rods positioned on a pitch of 2.032cm. The overall length of the rods was 97.79cm, of which 91.44cm was the fuel length. Each rod had an outer clad radius of 0.6350cm and a fuel radius of 0.5588cm.

The fuel clusters were located in a rectangular carbon-steel tank of wall thickness 0.952cm and of external dimensions 180.0cm x 300.0cm and height 210.0cm. The tank also contained a set of grid plates, a control blade, a safety blade, a water dump valve and associated electronic detection devices. The fuel clusters were supported by an acrylic plate located on aluminium 'U' shaped plinths positioned at the bottom of the tank. The electronic equipment was located at the periphery of the fuel rod clusters to prevent it perturbing the measurements.

The experiments selected for this validation study employed clusters comprising 17 x 20 fuel rods, with the following neutron absorbing materials:

- boral plates (experiment nos. 020 and 016)
- 304L steel plates with:

0% boron by weight (experiment nos. 034 and 035)
1.05% boron by weight (experiment nos. 032 and 033)
1.62% boron by weight (experiment nos. 038 and 039)

- no neutron absorbing plates (experiment no. 015)

These nine experiments have been given case numbers 1.01 to 1.09 respectively. Details of the critical separation distances X and G and the absorbing plate thicknesses (T) are given in Table 5.1.1.

5.1.2 The MONK Model

The MONK models of the experiments have been constructed from the data presented in Reference 3. However, some ambiguity and lack of clarity has meant that the following minor approximations and assumptions have had to be made:

(i) Temperature Effects

Standard room temperature modelling at 293K has been employed for Doppler broadening all reaction cross-sections. The actual temperature distribution of the experimental apparatus is not recorded, but it could not have departed sufficiently from 293K to affect the results of this study. However the effect has been assessed by performing a sensitivity study.

(ii) Acrylic Plates

Acrylic plates were used in the experiments as the supporting structure for the fuel clusters at three positions. The upper plates are grid plates of thickness 1.27cm, and are located in the vicinity of the bottom and top of the fuel elements; however the exact positions of the plates are not given in the experimental report. The lower plate is a solid support plate of thickness 2.54cm and is located on top of the aluminium plinth.

The composition of the acrylic material is not provided, and the experimentalists argue that the plates can be accurately represented as water due to its almost identical moderating characteristics; this is entirely reasonable as the plates constitute a small proportion of the total volume of moderator. Based on this recommendation the upper acrylic plates have been replaced by water in the MONK model, due to the uncertainty about their position. However as the position of the lower plate is known, it has been modelled assuming a typical acrylic atomic composition (see Table 5.1.2). The effect of omitting the upper acrylic plates has been assessed by performing a sensitivity study.

(iii) Aluminium Rods

Aluminium spacer/support rods 1.27cm diameter and 83.9cm long were positioned at each corner of the fuel clusters, although the exact locations are not given in the experimental report. Measurements made by the experimentalists demonstrated that the aluminium safety and control guide blades had no impact on the critical separation measurements. As these are of larger volume than the aluminium rods and are closer to the fuel rod clusters, it can be concluded that the aluminium rods would also have no effect. Therefore the aluminium rods have been omitted from the MONK model and replaced by water.

(iv) Aluminium Plates

Aluminium 'L' shaped plates 5.08cm x 5.08cm x 0.635cm were positioned at the top-end of the fuel elements to provide further support for the fuel clusters; their exact

positions are not given in the experimental report. An experimental sensitivity study, where the quantity of aluminium was doubled, demonstrated that the support plates did not effect the critical separation measurements. Therefore these plates have been omitted from the MONK model and replaced by water.

(v) Water

H_2O with a density 0.9982g/cm³ [8] has been employed in the MONK model. As stated above the effect of density changes arising from temperature changes has been assessed by performing a sensitivity study. All measured trace elements have been included in the water specification employed in the MONK model. The uncertainties quoted on the trace element concentrations have been ignored as the quantities involved are negligibly small.

(vi) Absorbing Plates

The dimensions of the absorbing plates are given in the experimental report but their axial positions are not, although it is stated that the plates were slightly longer and wider than the rod clusters (note that the boral plates and the steel plates are slightly different in width). Based on this information the plates have been modelled to extend beyond the fuel length and fuel cluster width equally in each direction. The difference between this and any alternative location that met the description given in the experimental report would be negligible. The composition of the plates was taken from the experimental report. (Note - for the boral plates, the element Zn is not present in the MONK continuous energy nuclear data library. However as its weight fraction is very small it has been replaced by Al27, in keeping with common experimental practice [9]).

(vii) Steel Tank

The composition of the carbon-steel tank is not given in the experimental report. It has been modelled as iron even though the experimentalists demonstrated that materials outside the reflector have negligible effect on the measured critical separation distances.

(viii) Safety and Control Components

The safety and control mechanisms are depicted in the experimental report to have been located in air above the water. The safety and control blades are fully withdrawn during measurements, presumably in the air above the water. It is therefore concluded that the safety and control mechanisms and blades are sufficiently well separated from the fuel rod clusters by the water to have a negligible effect on the critical separation measurements - they have therefore been omitted from the MONK model. The safety and control blade guides are made of aluminium and are permanently in place in the water between the fuel rod clusters. Experiments were performed where the aluminium thickness was doubled and these demonstrated no impact on the critical separation measurements. The safety and control blade guides have therefore also been omitted from the MONK model and replaced by water.

(ix) Additional Uncertainties

In addition to the sensitivity calculations mentioned above, calculations have also been performed to consider the following uncertainties in the MONK model: U235 enrichment, pin pitch, fuel clad outer diameter, fuel diameter, fuel density, and uranium isotopic composition. These are considered to provide the most significant uncertainty on the system multiplication [9].

Uncertainties on the critical separation distances and absorbing plate thicknesses are provided in the experimental report and sensitivity calculations have also been

performed to assess these. It has been assumed that the quoted uncertainties on these dimensions are simply measurement uncertainties and include no allowance for any other uncertainty.

Figures 5.1.1,5.1.2 and 5.1.3 show views of the MONK model geometry and present the important dimensions. The materials used in the MONK model are presented in Table 5.1.2. Each calculation employed 1000 neutrons per stage and was run to achieve a precision of smaller than 0.0015. This ensured that adequate statistical sampling was performed, which was verified by performing detailed checking of the output. The input specification and output for each calculation were independently checked. The results from two calculations using different random number seeds were averaged for each experiment to give a combined statistical precision of 0.0010.

5.1.3 Results

(a) Standard Calculations

MONKDEV calculations have been performed as described above using the values of the critical separation distances G and X and the plate thicknesses T given in Table 5.1.1. The results obtained from the calculations are summarised in Table 5.1.3.

The calculations indicate that the Monte Carlo code MONKDEV predicts the system multiplication for low-enriched UO_2 fuel pins with water moderator and reflector, and with boral, steel and boron-steel absorber plates, to within an accuracy of $\pm 0.11\%$; a similar result is observed for the system without absorber plates. However an analysis of the experimental uncertainties is required to assess the significance of this accuracy - this is considered below.

The mean value from the nine experiments is 1.0004 with a standard error of 0.0002. For the 18 MONKDEV runs, the observed external standard deviation is 0.0012 ± 0.0002 which is in good agreement with the estimated internal standard deviation of about 0.0014. This is a good check that 1000 superhistories per stage is adequate for settling to be established below the random noise level. There is no significant evidence of added statistical noise, despite the fact that the MONKDEV calculations represent nine different configurations. This suggests that the experimental measurements are of high quality and there is little or no drift in the MONKDEV bias between the configurations.

(b) Sensitivity Analysis

The effects of the various uncertainties have been examined to assess whether the above indication of the accuracy of the code is sustainable. Both the calculation and the experiment have residual errors/uncertainties that might affect the calculated value of k-effective. It is considered that the MONK model has been constructed with sufficient accuracy and the Monte Carlo sampling is adequate; therefore any deviations between the calculated and measured results are due either to errors/uncertainties in the nuclear data library used in the calculations or errors/uncertainties in the experiments. The experimental report quotes random reproducibility uncertainties, but the systematic uncertainties must be assessed by sensitivity analysis.

The first stage of the sensitivity analysis consisted of performing additional MONK calculations in order to assess the sensitivity of the system multiplication to the uncertainties in the separation distances X and G and the plate thickness T quoted in the experimental report. One boral-poisoned system, one boron-steel poisoned system and the unpoisoned system were selected for this sensitivity study.

Consequently experiments 1.01, 1.08 and 1.09 have been modified to provide the input for independent sensitivity calculations, each considering ten standard deviation increases in the relevant parameters (i.e. $T+10\sigma$, $G+10\sigma$ and $X+10\sigma$). The results from these calculations have

then been divided by ten to estimate the change in reactivity resulting from a one standard deviation increase; the linear relationship assumed is considered sufficiently accurate for the purpose.

In addition a calculation was performed to evaluate the effect of the uncertainty in the boron composition of the plates for the case with the largest relative uncertainty (304L steel with 1.05% boron). Consequently experiment 1.05 has been modified to provide the input for a sensitivity calculation considering a one standard deviation decrease in boron content.

The results for these calculations are summarised in Table 5.1.4, where it can be seen that the predicted reactivity changes are not significant compared with the calculated uncertainties. Therefore a one standard deviation experimental uncertainty of 0.0015 (0.15%) covers the effect of the uncertainties on the parameters considered in this part of the sensitivity study.

The second stage of the sensitivity analysis consisted of calculations to investigate the effect of the uncertainties on various other parameters that may make a significant contribution to the total experimental uncertainty. The selection of the parameters to investigate is based on the findings of the analysis of similar experiments performed in the DIMPLE reactor at Winfrith [9]. The calculations have been performed using the LWRWIMS code [10] for the case with no poison plates and with infinite length fuel pins, and the results obtained have been used to provide an estimate of the upper bound of the total experimental uncertainty for the whole range of configurations. The results for the parameters that have been studied are shown in Table 5.1.5.

Note that the uncertainties ascribed to the U235 enrichment, the cladding outer diameter, the fuel outer diameter and the uranium composition have been taken from the experimental documentation. A possible difference of ±5K between the standard MONK temperature and the experimental temperature has been considered, together with the associated density change to the moderator and reflector. The effect can be seen to be negligible. The results when added quadratically provide an upper bound of the total uncertainty for the listed parameters of 0.0017 (0.17%).

Finally it should be noted that MONK uses only the prompt neutron fission spectrum. The significance of delayed neutrons needs to be considered, so WIMS calculations have been carried out to assess their effect [11]. For the case without absorber plates (1.09) the change in the calculated k-effective was +0.00065, to which an uncertainty of 10% should be attributed to allow for differences between the prompt fission spectra employed in WIMS and MONK.

Summing the uncertainties from both parts of the sensitivity analysis quadratically to provide an upper bound to the total experimental uncertainty gives k-effective = 1.0000±0.0023. This can be compared with the calculated mean value of 1.0004±0.0002, to which a correction of 0.0006±0.0001 should be added to allow for the delayed neutron effect. Thus the difference between experiment and calculation is not significant even at the one standard deviation level.

(c) Comparison with MONK6B

Table 5.1.6 gives a comparison of the results for the nine experiments for the JEF2.2 library used with MONKDEV as reported above and for the current standard UKNDL-based library used with MONK6B.

As reported above the mean value for the JEF2.2 library calculations is 1.0004±0.0002. The mean value for the UKNDL calculations is 1.0046±0.0004. The differences between the two libraries is significant at the three standard deviation level, with the JEF-based library apparently providing better agreement with the experimental measurements. In each case the JEF2.2/MONKDEV result is closer to the experimental result than the UKNDL/MONK6B result. However the difference between the UKNDL calculations and experiment is not significant at the three standard deviation level.

5.1.4 Summary

This section has shown that the Monte Carlo code MONKDEV in conjunction with a JEF2.2-based nuclear data library calculates the mean system multiplication for a series of critical experiments using low-enriched UO_2 fuel pins with water moderator and reflector, and with boral, steel and boron-steel absorber plates, within 0.04%±0.02% of unity. Correcting for the effect of delayed neutrons does not significantly alter this result. The calculated deviation from unity compares with an estimated total experimental error of 0.23% (1σ). Thus the apparent small positive bias on the mean calculated value is not statistically significant even at the one standard deviation level and could be due solely to experimental errors/uncertainties.

Table 5.1.1 - MEASURED CRITICAL SEPARATION DISTANCES

Case No.	Exp. No.	Absorber Material	Absorber Plate Thickness (T) cm	Distance between Plates and Fuel (G) cm	Fuel Cluster Separation Distance (X) cm
1.01	020	Boral	0.713 ± 0.011 *	0.645 ± 0.006	6.34 ± 0.02
1.02	016	Boral	0.713 ± 0.011 *	4.442 ± 0.060	9.03 ± 0.05
1.03	034	304L Steel (no boron)	0.302 ± 0.013	0.645 ± 0.006	10.44 ± 0.03
1.04	035	304L Steel (no boron)	0.302 ± 0.013	4.042 ± 0.070	11.47 ± 0.03
1.05	032	304L Steel (1.05% boron)	0.298 ± 0.006	0.645 ± 0.006	7.56 ± 0.02
1.06	033	304L Steel (1.05% boron)	0.298 ± 0.006	4.042 ± 0.070	9.62 ± 0.03
1.07	038	304L Steel (1.62% boron)	0.298 ± 0.005	0.645 ± 0.006	7.36 ± 0.03
1.08	039	304L Steel (1.62% boron)	0.298 ± 0.005	4.042 ± 0.070	9.52 ± 0.03
1.09	015	None	-	-	11.92 ± 0.04

* includes 0.102cm Aluminium coating on each surface

Table 5.1.2 - SUMMARY OF MATERIAL DATA

Material	Density g/cm³	Nuclides Present	Fractions by Atom or Weight
UO_2 - 2.35% enriched-by-weight (1) (by atom)	9.20	U235 U238 O	2.3790E-02 9.7621E-01 2.0000E+00
Aluminium (by weight)	2.692	Al27 (2) Cr Cu Fe Mn Si Ti S32 (3)	9.7150E-01 2.1000E-03 1.2000E-03 8.2000E-03 2.1000E-03 8.2000E-03 6.1000E-03 6.0000E-04
Water (by weight)	0.9982 (4)	HinH2O O Cl N Cr Al27 (2) Mn Pb F19 (5) Fe Cu Cd S32 (3)	1.1188E-01 8.8809E-01 2.6000E-05 5.0000E-08 3.0000E-08 4.0000E-07 1.0000E-06 2.0000E-08 2.0000E-07 6.0000E-08 6.0000E-08 4.0000E-09 3.0000E-06
Acrylic (6) (by atom)	1.20	HinH2O (7) O C	8.00000E+00 2.00000E+00 5.00000E+00
Iron (by weight)	7.86	Fe	1.00000E+00

Table 5.1.2 - SUMMARY OF MATERIAL DATA (continued)

Material	Density g/cm³	Nuclides Present	Fractions by Atom or Weight
Boral (by weight)	2.49	Al27 (2) (10)	6.2490E-01
		B10 (8)	5.2900E-02
		B11	2.3410E-01
		C	7.9700E-02
		Cr	5.0000E-04
		Cu	9.0000E-04
		Fe	3.3000E-03
		Mg	5.0000E-04
		Mn	5.0000E-04
		Ni	2.0000E-04
		Si	2.0000E-03
		Na23 (9)	2.0000E-04
		S32 (3)	3.0000E-04
304L Steel (no boron) (by weight)	7.930	Cr	1.8560E-01
		Cu	2.7000E-03
		Fe	6.8240E-01
		Mn	1.3800E-02
		Mo	2.6000E-03
		Ni	1.1090E-01
304L Steel (1.05% boron) (by weight)	7.900	Cr	1.9030E-01
		Cu	2.8000E-03
		Fe	6.8040E-01
		Mn	1.5800E-02
		Mo	4.9000E-03
		Ni	9.5300E-02
		B10 (8)	1.9000E-03
		B11	8.6000E-03
304L Steel (1.62% boron) (by weight)	7.770	Cr	1.9600E-01
		Cu	2.6000E-03
		Fe	6.6400E-01
		Mn	1.6900E-02
		Mo	3.1000E-03
		Ni	1.0120E-01
		B10 (8)	3.0000E-03
		B11	1.3200E-02

Notes on Table 5.1.2

(1) Fuel impurities have been ignored. The effect of omitting U234 and U236 has been included in the sensitivity analysis; any other impurities are considered negligible. Atom ratios have been calculated using atomic weights contained in MONK nuclear data library.

(2) The MONK nuclide is Al27 which has a natural abundance of 100% [8].

(3) The MONK nuclide is S32 which has a natural abundance of 95% [8] - the difference is negligible at the low concentration present.

(4) Density of water is taken from Reference 8.

(5) The MONK nuclide is F19 which has a natural abundance of 100% [8].

(6) Acrylic composition taken from experimental documentation.

(7) The MONK nuclide HinH2O is recommended for all occurrences of bound hydrogen [1].

(8) The boron composition is taken from Reference 8.

(9) The MONK nuclide is Na23 which has a natural abundance of 100% [8].

(10) Zinc is not present in the MONK nuclear data library. In very low concentrations it can be accurately modelled as aluminium [9]. The aluminium weight fraction used here includes the Zinc weight fraction given in the experimental report.

Table 5.1.3 - RESULTS FROM STANDARD MONK CALCULATIONS

Case No.	Experiment No.	k-effective - run 1	k-effective - run 2	Mean k-effective
1.01	020	0.9992 (0.0014)	1.0020 (0.0014)	1.0006 (0.0010)
1.02	016	1.0012 (0.0014)	0.9990 (0.0014)	1.0001 (0.0010)
1.03	034	1.0016 (0.0015)	1.0003 (0.0015)	1.0010 (0.0010)
1.04	035	0.9989 (0.0014)	0.9995 (0.0014)	0.9992 (0.0010)
1.05	032	1.0010 (0.0015)	0.9978 (0.0014)	0.9993 (0.0010)
1.06	033	1.0011 (0.0014)	1.0004 (0.0015)	1.0008 (0.0010)
1.07	038	0.9998 (0.0014)	1.0013 (0.0015)	1.0005 (0.0010)
1.08	039	1.0017 (0.0014)	1.0002 (0.0014)	1.0010 (0.0010)
1.09	015	1.0012 (0.0014)	1.0009 (0.0015)	1.0011 (0.0010)

The figure in brackets for the individual calculations is the standard deviation estimated by MONKDEV. For the mean value the figure in brackets is the standard error on the mean value computed using the standard deviations from the two independent calculations.

Table 5.1.4 - RESULTS FROM MONK SENSITIVITY CALCULATIONS

Case No.	Experiment No.	uncertainty in k-effective (Δk) from 1σ change
1.01	020	
1.01A	020 (T+10σ)	0.0002 (0.0001)
1.01B	020 (G+10σ)	0.0000 (0.0001)
1.01C	020 (X+10σ)	0.0000 (0.0001)
1.08	039	
1.08A	039 (T+10σ)	0.0001 (0.0001)
1.08B	039 (G+10σ)	0.0001 (0.0001)
1.08C	039 (X+10σ)	0.0001 (0.0001)
1.09	015	
1.09A	015 (X+10σ)	0.0004 (0.0001)
1.05	032	
1.05A	032 (1σ reduction in boron content)	0.0009 (0.0015)

The figure in brackets in the mean k-effective column is the standard error on the mean value computed using the standard deviations from two independent calculations. The difference is computed by subtracting the reference case multiplication and scaling if appropriate. The resulting standard error given in brackets.

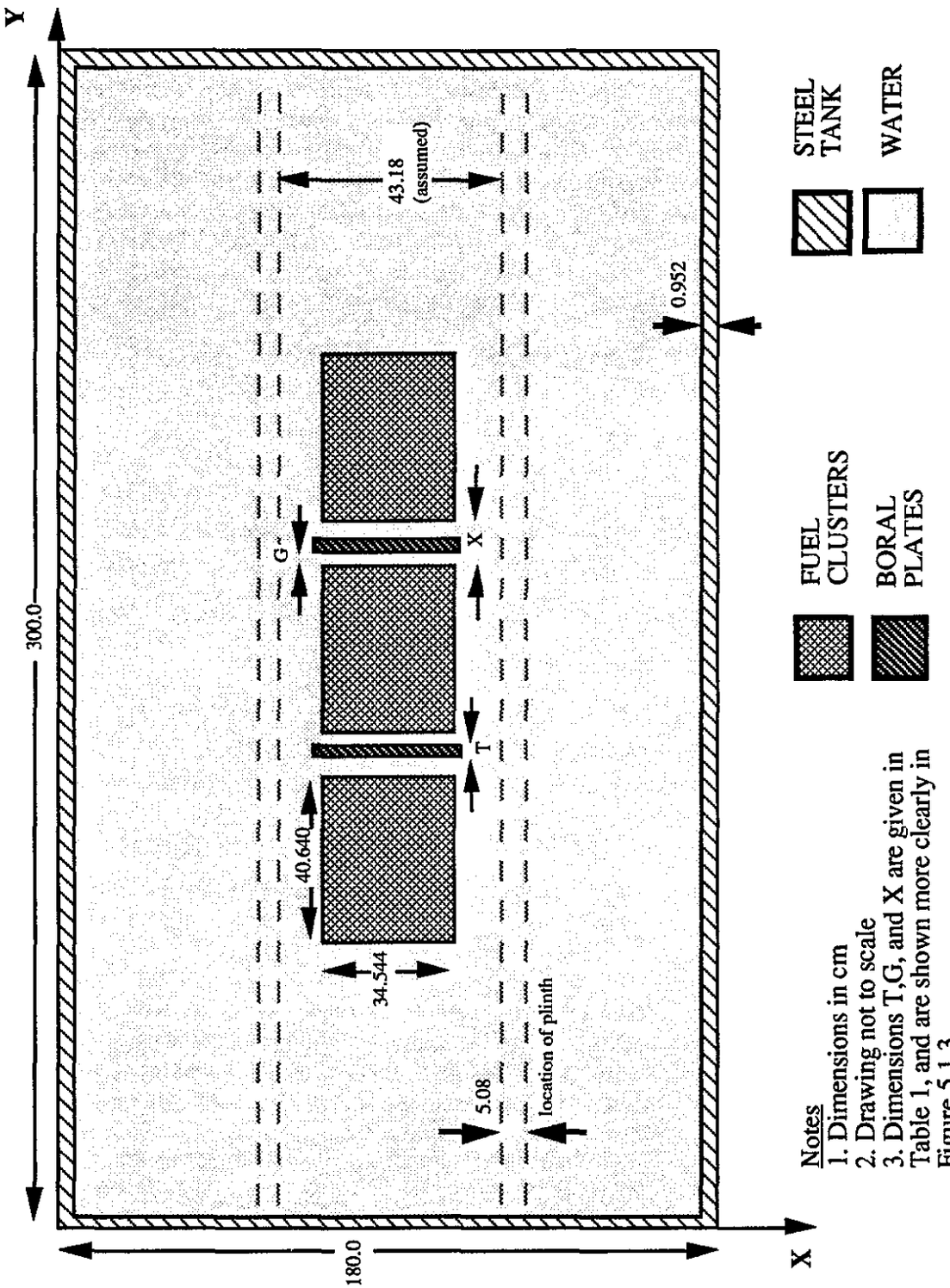
Table 5.1.5 - RESULTS FROM LWRWIMS SENSITIVITY CALCULATIONS

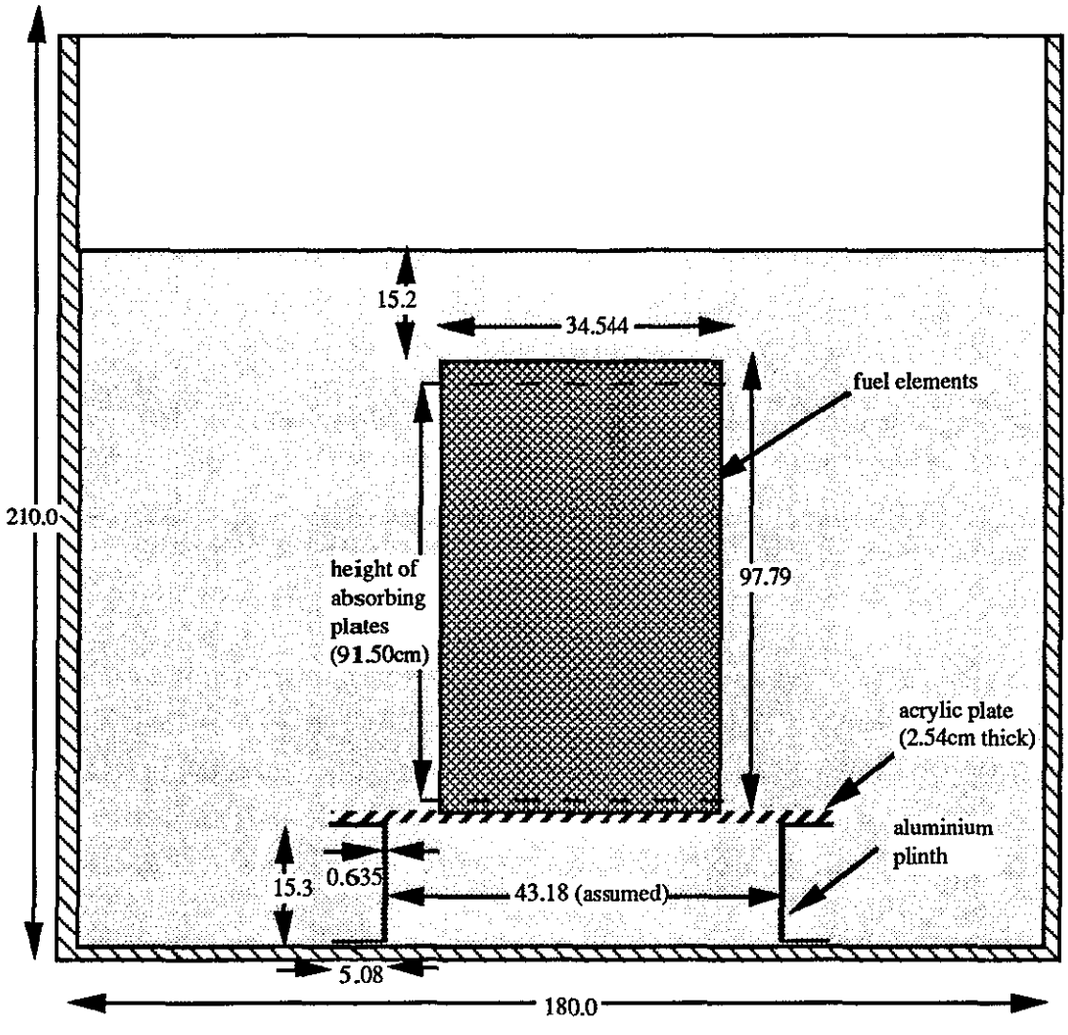
Parameter	parameter uncertainty	LWRWIMS-predicted uncertainty in k-effective (Δk)
U235 enrichment	0.003%	0.00034
Pin pitch (random uncertainty in last significant figure)	0.0005cm	0.00004
Cladding outer diameter	0.002cm	0.00036
Fuel outer diameter	0.003cm	0.00089
Temperature	5K	0.00001
UO_2 density (random uncertainty in last significant figure)	0.005g/cm^3	0.00010
Acrylic plates (acrylic comprising 3% of moderator volume)	displacement of water	0.00100
Uranium composition	inclusion of U234 and U236	0.00103

Table 5.1.6 - COMPARISON WITH MONK6B

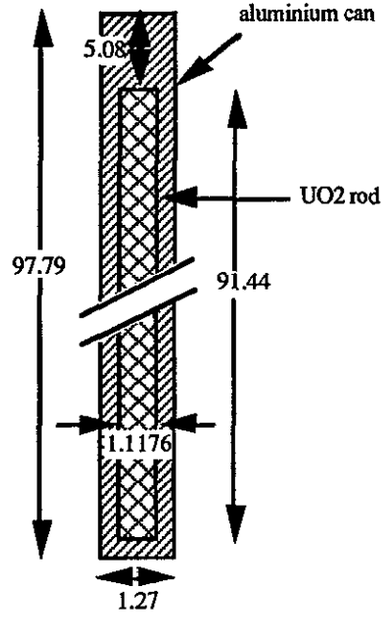
Case No.	Mean k-effective - JEF2.2/MONKDEV	Mean k-effective - UKNDL/MONK6B
1.01	1.0006 (0.0010)	1.0045 (0.0010)
1.02	1.0001 (0.0010)	1.0041 (0.0010)
1.03	1.0010 (0.0010)	1.0051 (0.0010)
1.04	0.9992 (0.0010)	1.0030 (0.0010)
1.05	0.9993 (0.0010)	1.0053 (0.0010)
1.06	1.0008 (0.0010)	1.0042 (0.0010)
1.07	1.0005 (0.0010)	1.0038 (0.0010)
1.08	1.0010 (0.0010)	1.0039 (0.0010)
1.09	1.0011 (0.0010)	1.0076 (0.0010)

Figure 5.1.1 - PLAN VIEW OF THE MONK MODEL





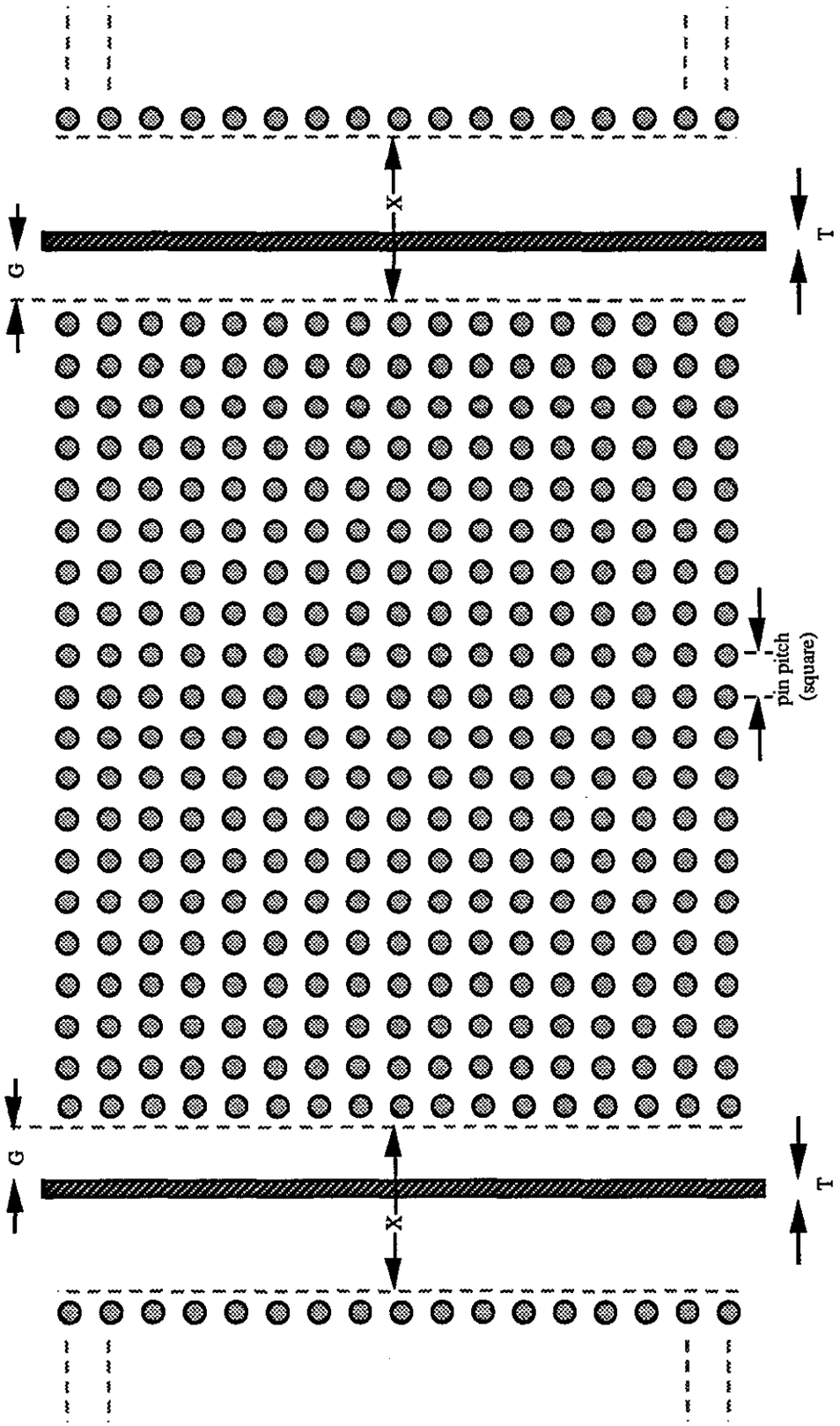
ENLARGED VIEW OF FUEL ELEMENT



Notes
1.Dimensions in cm
2.Drawing not to scale

Figure 5.1.2 - SECTIONAL VIEW OF THE MONK MODEL

Figure 5.1.3 - DETAILED PLAN VIEW OF THE CENTRAL FUEL CLUSTER



Notes
1. Drawing not to scale
2. See Figure 5.1.1 for overall plan view

5.2 Experiment Number 2

5.2.1 Experimental Description

The experimental programme from which the experiments were selected [4] was carried out at the Valduc Critical Mass Laboratory during the late 1970's for the Commissariat à l'Energie Atomique Department of Nuclear Safety.

The experimental programme considered water moderated and reflected arrays of low-enriched UO_2 fuel rods on various square and triangular pitches, and the effect of pin removal in under-moderated square pitch lattices. The aim of the programme was to provide data for validating techniques and nuclear data used in criticality assessments of LWR-type fuel element storage and transportation.

The experimental configuration comprised an array of LWR-type fuel rods within a large tank containing water, with reactivity controlled by means of water moderator level alone. The fuel rods were supported by two grid plates containing holes of pitch appropriate to the experiment; these grid plates were in turn attached by tie rods to a support plate.

The fuel used in the experiments was 4.742% by weight U235 enriched UO_2 rods clad in aluminium alloy (type AG5). The fuel length was 90cm, with an overall rod length of 100cm. Each rod had an outer clad radius of 0.47cm, an inner clad radius of 0.41cm and a fuel radius of 0.395cm.

The nine assemblies chosen for this study as being representative of the experimental programme comprised three arrays with different square pitches (corresponding to under-, optimum- and over-moderation), three arrays with different triangular pitches, and three arrays with the same square under-moderated pitch but with differing numbers of fuel pins removed. The three triangular pitches provided equivalent levels of moderation (i.e. the same fuel to moderator ratios) to the three square pitches. Details of the fuel pin arrangements are shown in Figure 5.2.3.

The critical water height was measured by the experimentalists for each assembly. This was performed by extrapolating the inverse count-rates recorded during a progressive rise in water level, with the water acting as both moderator and reflector. The critical height measurement was determined from a linear extrapolation of two consecutive points. The measured critical heights are given in Table 5.2.1 where these are distances from the bottom of the fuel column and are based on the average of five detector measurements. The uncertainty in the measured heights is said to include:

(i) a variable uncertainty, which was the standard deviation between the individual extrapolations and their average value. This was always <0.05cm.

(ii) a systematic uncertainty of 0.05cm that resulted from the accuracy of the height measuring equipment.

However, investigations by the experimentalists into the reproducibility of the critical height following an unload and reload of the critical assembly showed a total error of ±0.2cm and it is this value that has been used in the sensitivity calculations for these experiments.

5.2.2 The MONK Model

The MONK models of the experiments have been constructed from the data presented in the experimental reference [4]. However some ambiguity and lack of clarity has meant that the following minor approximations and assumptions have had to be made:

(i) Temperature Effects

Standard room temperature modelling at 293K has been employed for Doppler broadening all reaction cross-sections, whereas the actual temperature of the experimental apparatus is quoted as 295K. The effect of this difference has been assessed by performing a sensitivity study.

(ii) Water

For the temperature of 295K quoted for all experiments, the corresponding water density is 0.9978g/cm^3 [8]. The effect of a change in density caused by an assumed maximum measurement uncertainty of about 1K has been assessed by sensitivity calculations described later. No water impurity data are available, therefore pure water has been assumed. In comparable experiments performed in the DIMPLE reactor at Winfrith [9], the moderator impurities were shown to have a negligible effect on the system multiplication (<0.000005).

(iii) Cladding

The fuel is maintained within the cladding by a spring in the upper plenum. The dimensions and composition of the spring are not recorded in the experimental reference. Therefore, the spring was omitted from the model and the 6.9cm region above the fuel was represented as void. There are only two cases where this could have a significant effect, namely cases 2.01 and 2.09 where the critical moderator heights were within and approaching the spring region respectively. To assess the effect of omitting the spring, a further calculation was performed modelling the spring region as solid stainless steel. This over-estimate of the situation provides an upper bound calculation. The remainder of the cladding is quoted as Aluminium alloy (type AG5) with a density of 2.7g/cm^3.

(iv) Support Plate and Grid

The exact axial location of the upper support grid is not given in the experimental report but is quoted as having a negligible effect on reactivity due to its small dimensions and location close to the top of the fuel pins above the water level. The upper support grid has therefore been omitted from the MONK model and replaced by void.

Only the thicknesses of the lower support plate and grid are provided in the experimental report, although the drawings show the lattice grid as being the full width of the fuel array and the support plate as being the full width of the experimental tank. Any minor differences between the drawings and the actual arrangement will have a negligible effect on the reactivity due to the small quantity of material involved and its location relative to the fuel. The stainless steel is quoted as French Standard Type Z3 CN 18 10, with a density of 7.9g/cm^3.

(v) Experimental Tank, Steel Tie Rods and Support Feet

The exact locations of these items are not provided in the experimental report but, due to their small size and distance from the fuel rods (separated by more than 20cm of water), their omission from the calculation is not significant in terms of reactivity.

(vi) Additional Uncertainties

In addition to the sensitivity calculations mentioned above, calculations have been carried out to assess the uncertainties associated with the U235 enrichment, pin pitch, fuel clad outer diameter, fuel diameter, fuel density and uranium isotopic composition specified in the MONK model. Based upon previous experience [9] these are considered to provide the most significant uncertainty on the system multiplication.

Figures 5.2.1 and 5.2.2 show views of the MONK model geometry and present the important dimensions. The materials used in the MONK models are given in Table 5.2.2. Each calculation employed 1000 neutrons per stage and was run to achieve a precision smaller than 0.0015. This ensured that adequate statistical sampling was performed, which was verified by performing detailed checking of the output. The input specification and output for each calculation were independently checked. The results from two calculations using different random number seeds were averaged for each experiment to give a combined statistical precision of about 0.0010.

5.2.3 Results

(a) Standard Calculations

MONKDEV calculations have been performed as described above using the critical water heights given in Table 5.2.1. The results obtained from the calculations are given in Table 5.2.3. The calculations indicate that MONKDEV overpredicts the system multiplication for low-enriched UO_2 fuel pins with water moderator and reflector by between 0.2% and 1.0%. However, an analysis of the experimental uncertainties is required to assess the significance of this over-prediction.

When considering the nine experiments as a whole the mean k-effective is 1.0057 with a standard error of 0.0008. The observed standard deviation for these eighteen cases is 0.0024 ±0.0004 compared with an internal standard deviation of 0.0015. To assess whether this difference is due to the calculated deviation from unity varying as a function of the moderator to fuel ratio, the experiments have been grouped as a function of pitch. Note that for each of the triangular pitches there is an equivalent square pitch case that has the same moderator to fuel ratio. It is this effective square pitch that has been used to include the triangular pitch cases into the moderator to fuel ratio categories corresponding to the three different square pitches.

The five experiments performed with the square pitch of 1.26cm, or the equivalent triangular pitch of 1.35cm, (cases 2.01, 2.04, 2.07, 2.08 and 2.09) give a mean k-effective of 1.0071 with a standard error of 0.0008. The two calculations performed with the square pitch of 1.60cm, or the equivalent triangular pitch of 1.72cm (cases 2.02 and 2.05), give a mean k-effective of 1.0051 with a standard error of 0.0004. The two calculations performed with the square pitch of 2.10cm, or equivalent triangular pitch of 2.26cm (cases 2.03 and 2.06), give a mean k-effective of 1.0028 with a standard error of 0.0009. The sensitivity analysis described below examines the experimental uncertainty for each pitch grouping.

(b) Sensitivity Analysis

The MONK models and the Monte Carlo sampling introduce negligible uncertainties. Any deviations between the calculated and measured results are therefore due either to errors/uncertainties in the nuclear data library used in the calculations or errors/uncertainties in the experiments.

Starting with the experimental uncertainties, these must be assessed by sensitivity analysis. The items chosen for study are those that arise from assumptions made in interpreting the experiments, from uncertainties measured by the experimentalists or from assumed uncertainties arising from the quoted precision of significant parameters.

The first stage of the sensitivity analysis consisted of additional MONK calculations to assess the sensitivity of the system multiplication to the uncertainties in the contents of the spring region and moderator height. The spring sensitivity calculation was performed for the case where the moderator partially flooded the spring region and the moderator sensitivity calculation was carried out for the optimum pitched case. These cases were chosen in order to produce the greatest effects for use as upper bounds on the uncertainties.

In the spring case, using experiment 2.01, the spring was modelled as solid stainless steel. This representation of the spring provides an over-estimate of its true worth and this has been estimated to be equivalent to a ten standard deviation uncertainty (at least). The moderator case, using experiment 2.02, considered an increase ten times greater than the one sigma uncertainty given in the experimental report. In each case the calculated effect was rescaled on the assumption of a linear relationship.

The results from these calculations are summarised in Table 5.2.4, where it can be seen that the predicted reactivity changes are not significant compared with the calculated uncertainties. However in order to accommodate the statistical uncertainty in the MONK sensitivity calculations, a one standard deviation experimental uncertainty of 0.0006 (0.06%) will be assigned to cover the effect of the uncertainties on the parameters considered in this part of the sensitivity study.

The second stage of the sensitivity analysis consisted of calculations to investigate the effect of the uncertainties on various other parameters that may make a significant contribution to the total experimental uncertainty. The selection of the parameters to investigate was based on the findings of the analysis of similar experiments performed in the DIMPLE reactor at Winfrith [9]. To provide the uncertainty analysis, calculations were performed with the LWRWIMS code [10] for a 2-D representation of each of the square pitch full lattice experiments. The results for the parameters studied are shown in the Table 5.2.5.

The results of the second stage of the uncertainty analysis when added quadratically provide an upper bound for the total experimental uncertainty for the listed parameters of 0.40% for the 1.26cm pitch case, 0.20% for the 1.60cm pitch case, and 0.16% for the 2.10cm pitch case. Note that the difference in the uncertainties for the three categories arises largely from the different relative importance of the precision of the pin pitch measurement. Including the uncertainties observed in the first stage of the sensitvity analysis leads to a total uncertainty of 0.40% for the 1.26cm pitch case, 0.21% for the 1.60cm pitch case, and 0.17% for the 2.10cm pitch case

Turning to the calculational uncertainty, firstly the calculations were performed at a temperature of 20°C, rather than the measured experimental temperature of 22°C. However, based on the experimental sensitivity calculations reported above this would result in a negligible correction to the calculated values.

Secondly it should be noted that MONK uses only the prompt neutron fission spectrum. The significance of delayed neutrons needs to be considered, so WIMS calculations have been carried out to assess their effect [11]. For the three different pitches of 1.26cm, 1.60cm and 2.10cm, the changes in the calculated values of k-effective were +0.00124, +0.00149 and +0.00122 respectively. Each of these changes in the calculated values of k-effective has been assigned an uncertainty of 10% to allow for differences between the prompt fission spectra employed in WIMS and MONK. The effect of this correction on the mean calculated values of k-effective is shown in Table 5.2.6.

In summary the combined experimental and calculational results and uncertainties given in Table 5.2.6 show that the over-prediction of calculation compared with experiment is significant at the three standard deviation level for only one of the three pitch categories. For the other two categories the over-prediction is significant at the two standard deviation level. The difference in over-prediction between the categories could be due solely to the difference in experimental uncertainty between the three cases.

(c) Comparison with MONK6B

Table 5.2.7 gives a comparison of the results for the nine experiments for the JEF2.2 library used with MONKDEV as reported above and for the current standard UKNDL-based library used with MONK6B.

As reported above the mean values for the JEF2.2 library calculations for the three pitch categories are 1.0071±0.0008, 1.0051±0.0004 and 1.0028±0.0009. The corresponding mean values for the UKNDL calculations are 1.0110±0.0006, 1.0097±0.0016 and 1.0048±0.0003. The differences between the two libraries is significant at the three standard deviation level for the first case only, but with the JEF-based library providing apparently better agreement with the experimental measurements in all three cases. In each case the JEF2.2/MONKDEV result is closer to the experimental result than the UKNDL/MONK6B result.

5.2.4 Summary

This section has shown that the Monte Carlo code MONKDEV in conjunction with a JEF2.2-based nuclear data library overpredicts the mean system multiplication for low-enriched UO_2 fuel pins with water moderator and reflector, by between 0.2% and 0.7%. Including a correction for the delayed neutron effect increases the over-prediction by about 0.15%. When the experimental uncertainty is taken into account this over-prediction is significant at the three standard deviation level for only one of the three pitch categories. For the other categories the over-prediction could be due solely to experimental uncertainties.

Table 5.2.1 - EXPERIMENTAL CRITICAL WATER HEIGHTS

Case No.	Pitch type	Pitch (cm)	Number of rods		Frequency of holes	Critical water height (cm)	Standard deviation (1σ)
			along edge	total			
2.01	square	1.26 (1)	22x22	484	-	90.69	0.10
2.02	square	1.60 (2)	16x17	272	-	73.53	0.10
2.03	square	2.10 (3)	15x15	225	-	77.98	0.06
2.04	triangular	1.35 (1)	14	547	-	60.93	0.06
2.05	triangular	1.72 (2)	10	271	-	68.06	0.06
2.06	triangular	2.26 (3)	9	217	-	79.50	0.06
2.07	square	1.26 (4)	22x22	459	1 in 5	81.36	0.07
2.08	square	1.26 (4)	22x22	363	1 in 2	58.77	0.06
2.09	square	1.26 (4)	21x21	392	1 in 3	89.07	0.07

Notes on Table 5.2.1

(1) Moderator to fuel ratio (Vm/Vu) = 1.82

(2) Moderator to fuel ratio (Vm/Vu) = 3.81

(3) Moderator to fuel ratio (Vm/Vu) = 7.58

(4) Moderator to fuel ratio (Vm/Vu) = 1.82 for pin cells with pins present

where Vm/Vu = volume of water in pin cell outside cladding/volume of UO_2 in pin cell

Table 5.2.2 - SUMMARY OF MATERIAL DATA

Material	Density g/cm³	Nuclides Present	Fractions by Atom or weight
UO_2 - 4.742% enriched (1) (by weight) [2]	10.38	U235 U238 O B10 (2) B11	4.179200E-02 8.395229E-01 1.186846E-01 9.000000E-08 4.100000E-07
Aluminium (AG5) (by weight) [2]	2.7	Al27 (3) Mg Si Fe	9.8880E-01 (4) 4.7000E-03 4.3000E-03 2.2000E-03
Water (by atom) [2]	0.9978 (5)	HinH2O O	2.0000E+00 1.0000E+00
Stainless Steel (Z3 CN 18 10) (by weight) [4]	7.9	Fe Cr Ni	7.1397E-01 (6) 1.9162E-01 0.9441E-01

Notes on Table 5.2.2

(1) Fuel impurities as reported in the experimental report have been included. The possible effect of omitting U234 has been included in the sensitivity analysis; any other impurities are considered negligible.

(2) The boron composition is taken from Reference 8.

(3) The MONK nuclide for Al is Al27 which has a natural abundance of 100% [8].

(4) The AG5 material contained 0.03% Zn and this has been included with the Al.

(5) Density of water is taken from Reference 8.

(6) The weight fractions for stainless steel in the experimental report sum to 99.99%. The values listed here are normalised to sum to 100% consistent with the normalisation performed by MONK.

Table 5.2.3 - RESULTS FROM STANDARD MONK CALCULATIONS

Case No.	Pitch (cm) (1)	k-effective - run 1	k-effective - run 2	Mean k-effective
2.01	1.26	1.0081 (0.0015)	1.0115 (0.0015)	1.0098 (0.0011)
2.02	1.60	1.0045 (0.0015)	1.0049 (0.0015)	1.0047 (0.0011)
2.03	2.10	1.0038 (0.0015)	1.0034 (0.0015)	1.0036 (0.0011)
2.04	1.26	1.0076 (0.0015)	1.0084 (0.0015)	1.0080 (0.0011)
2.05	1.60	1.0047 (0.0015)	1.0060 (0.0014)	1.0054 (0.0010)
2.06	2.10	1.0013 (0.0014)	1.0024 (0.0014)	1.0019 (0.0010)
2.07	1.26	1.0071 (0.0015)	1.0042 (0.0015)	1.0057 (0.0011)
2.08	1.26	1.0053 (0.0015)	1.0061 (0.0015)	1.0057 (0.0011)
2.09	1.26	1.0072 (0.0015)	1.0050 (0.0015)	1.0061 (0.0011)

The figure in brackets for the individual calculations is the standard deviation estimated by MONKDEV. For the mean value the figure in brackets is the standard error on the mean value computed using the standard deviations from the two independent calculations.

Notes on Table 5.2.3

(1) For the triangular pitch cases (2.04, 2.05, 2.06) the pitch given here is the effective square pitch which maintains the moderator to fuel ratio.

Table 5.2.4 - RESULTS FROM MONK SENSITIVITY CALCULATIONS

Case No.	Uncertainty considered	Uncertainty in k-effective (Δk) from 1σ change
2.01 2.01A	Solid stainless steel spring (assumed 10σ)	0.0003 (0.0002)
2.02 2.02A	2cm moderator height change (10σ)	0.0005 (0.0002)

The figure in brackets in the mean k-effective column is the standard error on the mean value computed using the standard deviations from two independent calculations. The difference is computed by subtracting the reference case multiplication and scaling. The resulting standard error is given in brackets.

Table 5.2.5 - RESULTS FROM LWRWIMS SENSITIVITY CALCULATIONS

Parameter	Parameter uncertainty	Uncertainty in k-effective (Δk)		
		Pitch = 1.26cm	Pitch = 1.60cm	Pitch = 2.10cm
U235 enrichment [4]	0.001%	0.00003	0.00004	0.00006
Pin pitch (random uncertainty in last significant figure)	0.005cm	0.00348	0.00134	0.00001
Cladding outer diameter (assumed same as fuel)	0.002cm	0.00111	0.00048	0.00018
Fuel outer diameter [4]	0.002cm	0.00032	0.00068	0.00109
Temperature (assumed uncertainty)	1K	0.00009	0.00008	0.00007
UO_2 density [4]	0.04g/cm^3	0.00033	0.00051	0.00073
Uranium composition (assumed uncertainty)	inclusion of U234	0.00151	0.00115	0.00089

Table 5.2.6 - COMPARISON OF CALCULATIONS AND EXPERIMENT

Pitch (1)	Mean Calculated Result	Mean Calculated Result (corrected for delayed neutron effect)	Experiment
1.26cm	1.0071±0.0008	1.0083±0.0008	1.0000±0.0040
1.60cm	1.0051±0.0004	1.0066±0.0004	1.0000±0.0021
2.10cm	1.0028±0.0009	1.0040±0.0009	1.0000±0.0017

Notes on Table 5.2.6

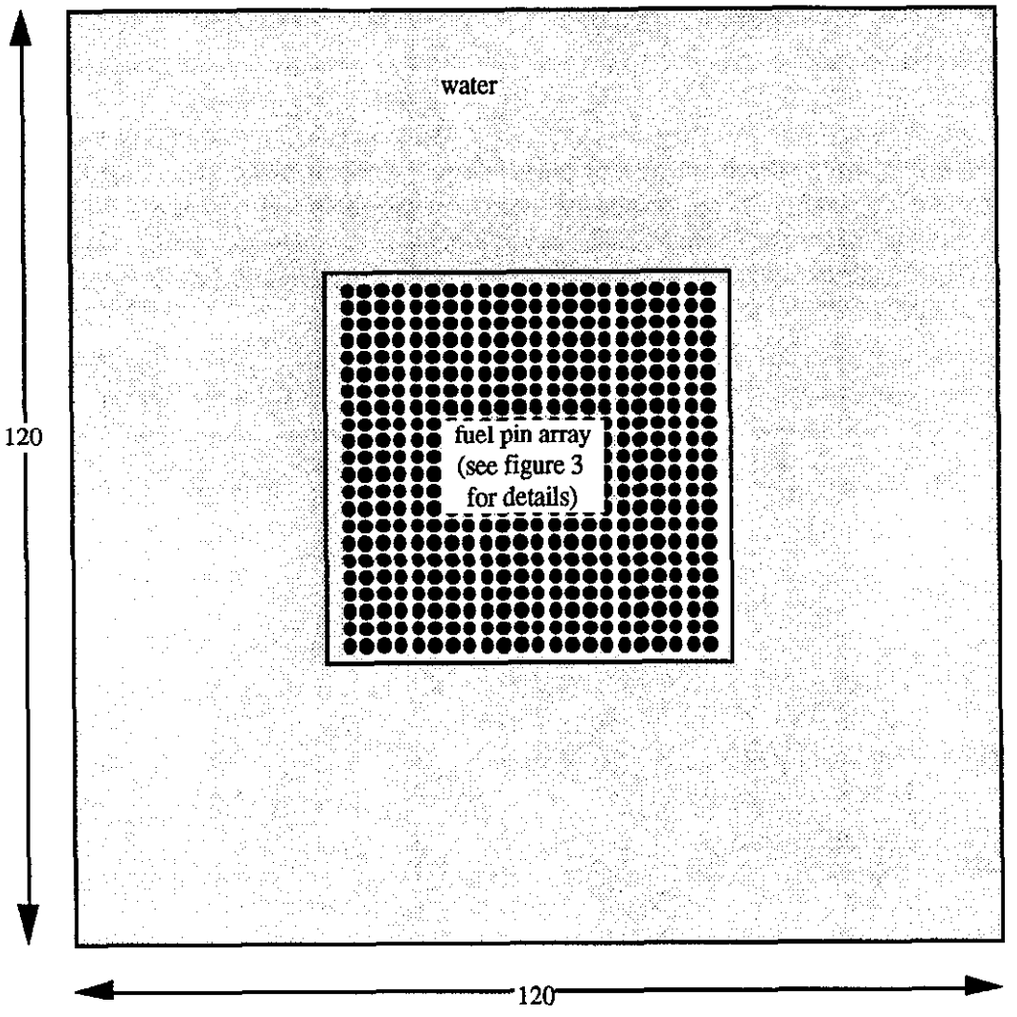
(1) The cases are grouped according to their effective square pitch (see Table 5.2.3).

Table 5.2.7 - COMPARISON WITH MONK6B

Case No.	Mean k-effective - JEF2.2/MONKDEV	Mean k-effective - UKNDL/MONK6B
2.01	1.0098 (0.0011)	1.0119 (0.0011)
2.02	1.0047 (0.0011)	1.0112 (0.0011)
2.03	1.0036 (0.0011)	1.0044 (0.0010)
2.04	1.0080 (0.0011)	1.0124 (0.0011)
2.05	1.0054 (0.0010)	1.0081 (0.0011)
2.06	1.0019 (0.0010)	1.0050 (0.0011)
2.07	1.0057 (0.0011)	1.0090 (0.0011)
2.08	1.0057 (0.0011)	1.0116 (0.0011)
2.09	1.0061 (0.0011)	1.0102 (0.0011)

The figure in brackets for the individual calculations is the standard error estimated by MONK.

Figure 5.2.1 - PLAN VIEW OF THE MONK MODEL



Notes
1.Dimensions in cm
2.Drawings not to scale

Figure 5.2.2 - SECTIONAL VIEW OF THE MONK MODEL

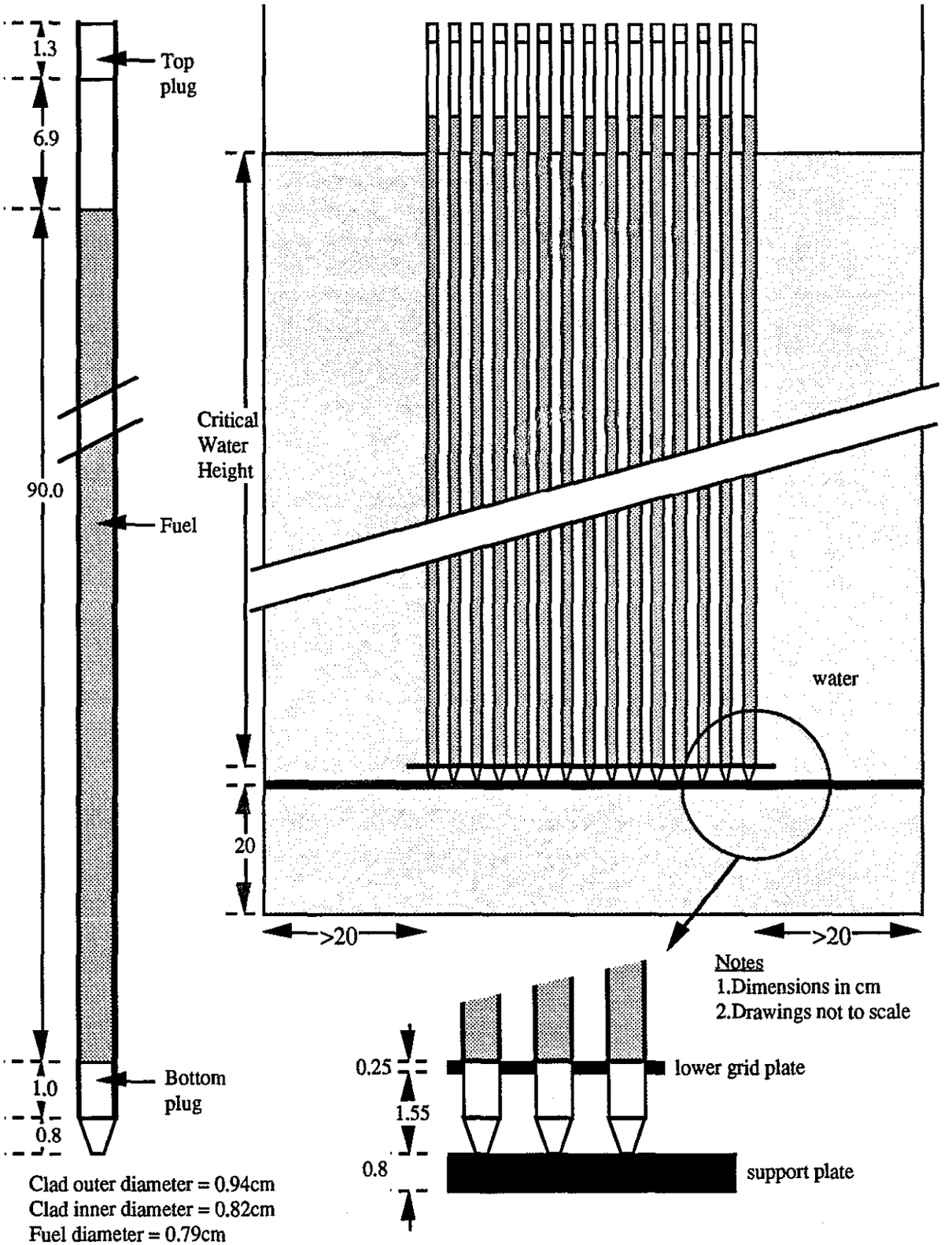
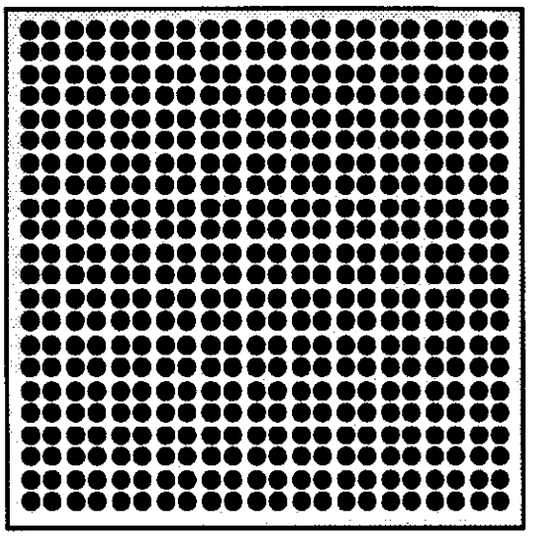
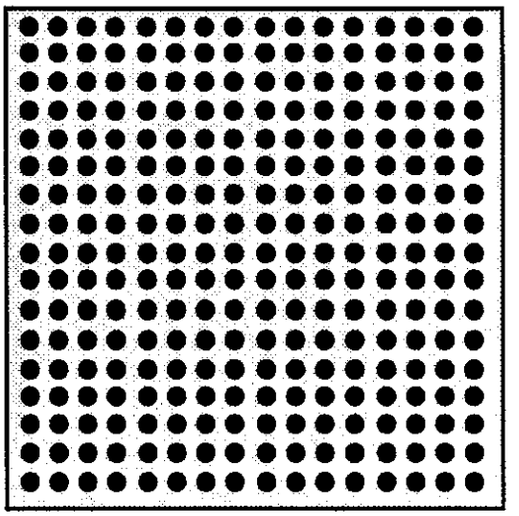


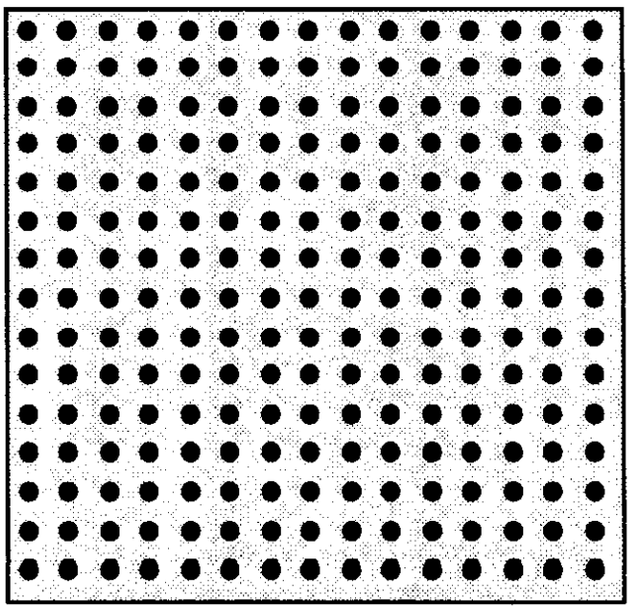
Figure 5.2.3 - PLAN VIEWS OF THE FUEL PIN ARRAYS



Case 1 - 22x22 pins - Pitch = 1.26cm

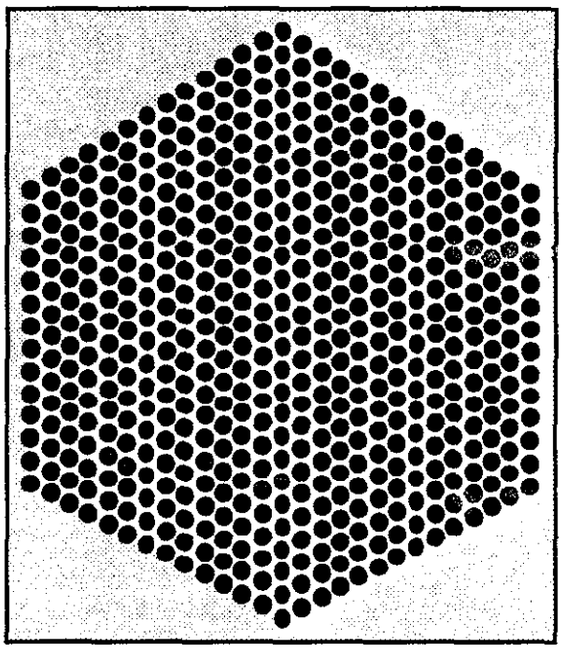


Case 2 - 16x17 pins - Pitch = 1.60cm

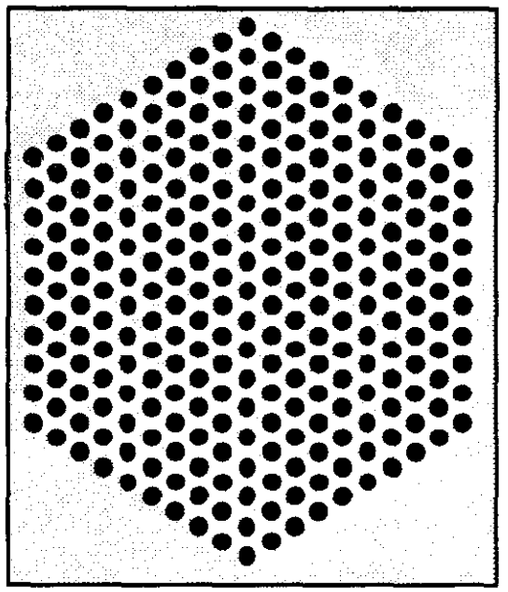


Case 3 - 15x15 pins - Pitch = 2.10cm

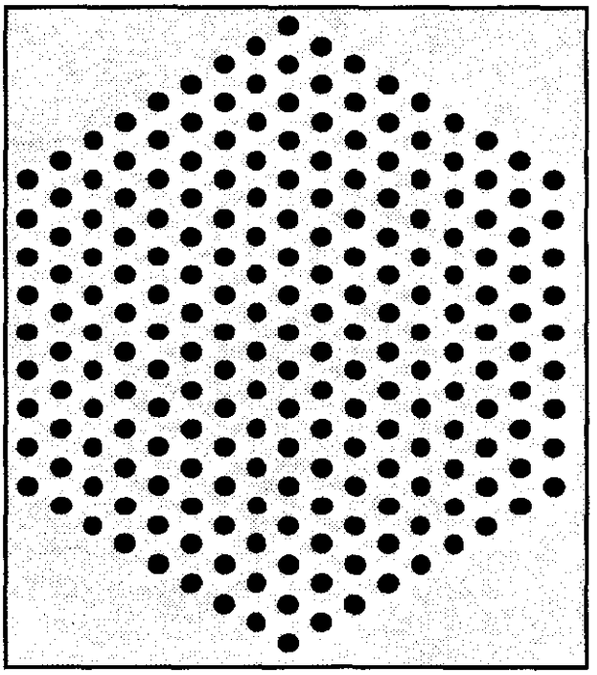
Figure 5.2.3 - PLAN VIEWS OF THE FUEL PIN ARRAYS (continued)



Case 4 - 14 pins per side - Pitch = 1.35cm

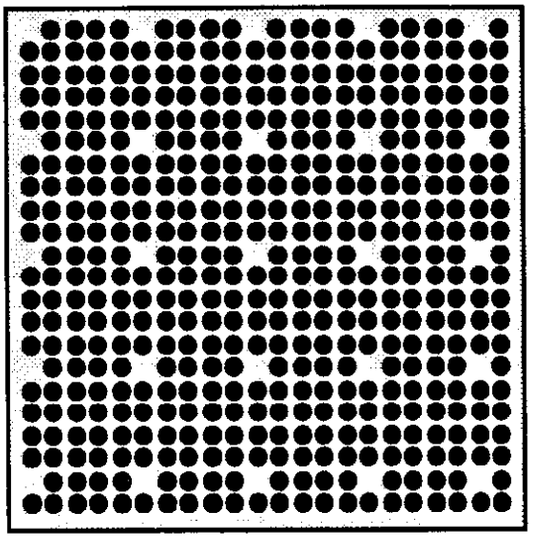


Case 5 - 10 pins per side - Pitch = 1.72cm

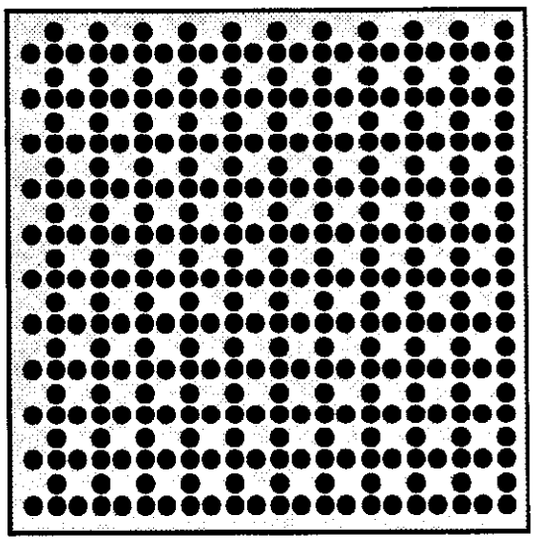


Case 6 - 9 pins per side - Pitch = 2.26cm

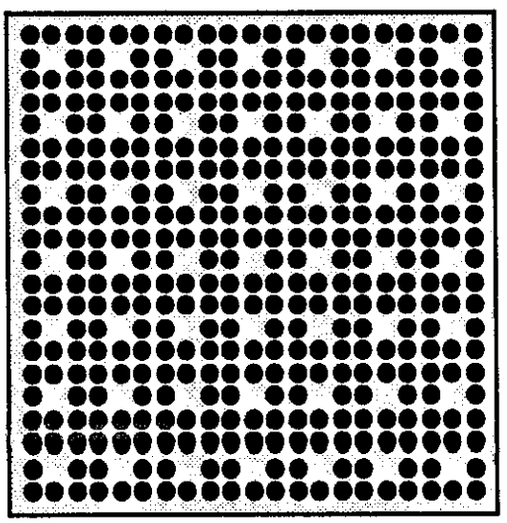
Figure 5.2.3 - PLAN VIEWS OF THE FUEL PIN ARRAYS (continued)



Case 7 - 22x22 pins - Pitch = 1.26cm
1 in 5 pins removed



Case 8 - 22x22 pins - Pitch = 1.26cm
1 in 2 pins removed



Case 9 - 21x21 pins - Pitch = 1.26cm
1 in 3 pins removed

5.3 Experiment Number 3

5.3.1 Experimental Description

The experimental programme from which the experiments were selected was performed at the Battelle PNL Critical Mass Laboratory [5] starting in 1976, with funding from the US Nuclear Regulatory Commission.

The experimental programme considered water moderated and reflected clusters of low-enriched UO_2 fuel rods, both with and without interspersed neutron absorbing materials in the form of plates. The aim of the programme was to provide data for validating methods of calculation and nuclear data used in criticality assessments of LWR-type fuel element transport packages and similar systems.

The experimental configuration comprised three clusters of LWR-type fuel rods within a large tank containing water. In most of the experiments a neutron-absorbing plate was located between the central cluster and each of the other two clusters. For a given cluster size, the separation distance between the clusters (X), and when present, the separation distance between the central cluster and the absorbing plates (G), acted as the experimental control mechanisms in the approach to critical.

Figures 5.3.1 and 5.3.2 give an overall view of the experimental configuration. Figure 5.3.3 gives an enlarged view of the central cluster, and shows more clearly the separation distances X and G. Note that the system is symmetrical with respect to the separation distances, and that the distances are measured to the edge of a notional fuel cell boundary.

The following range of neutron absorbing plates was employed in the experimental programme:

- 304 L Steel with 0.0, 1.05 and 1.62 wt% Boron
- Boral
- Copper with 0.0 and 1.0 wt% Cadmium
- Cadmium
- Aluminium
- Zircaloy-4

In addition some experiments were performed without the neutron absorbing plates.

The fuel used in all the experiments was aluminium-clad 4.31 Wt% U235 enriched UO_2 rods positioned on a pitch of 2.54cm. The overall length of the rods was 96.52cm, of which 91.44cm was the fuel length. Each rod had an outer clad radius of 0.7075cm and a fuel radius of 0.6325cm. The experimental report [5] quotes the fuel enrichment as 4.29 wt% U235 enriched UO_2 rods. However this figure was re-evaluated in 1980 to 4.31 wt%.

The fuel clusters were located in a rectangular carbon-steel tank of wall thickness 0.952cm and of external dimensions 180.0cm x 300.0cm and height 210.0cm. The tank also contained a set of grid plates, a control blade, a safety blade, a water dump valve and associated electronic detection devices. The fuel clusters were supported by an acrylic plate located on a pair of parallel aluminium 'U' shaped plinths positioned at the bottom of the tank. The cross-section of each of the plinths had outer dimensions of 5.08 x 15.3cm and was made of material 0.635cm thick; the plinths were separated by a distance of 43.18cm. The electronic equipment was located at the periphery of the fuel rod clusters to prevent it perturbing the measurements.

The experiments selected for this validation study employed clusters comprising 8 x 15 fuel rods, with the following neutron absorbing materials:

- no neutron absorbing plates

- 304L steel plates (35.6 x 91.5cm) with:

  0% boron by weight
  1.05% boron by weight
  1.62% boron by weight

- boral plates (36.5 x 91.5cm)

The eight experiments selected have been given MONK validation numbers 3.01 to 3.08. Details of the critical separation distances X and G and the absorbing plate thicknesses (T) are given in Table 5.3.1.

5.3.2 The MONK Model

The MONK models of the experiments have been constructed from the data presented in Reference 5. However, some ambiguity and lack of clarity has meant that the following minor approximations and assumptions have had to be made:

(i) Temperature Effects

Standard room temperature modelling at 293K has been employed for Doppler broadening all reaction cross-sections. The actual temperature distribution of the experimental apparatus is not recorded, but it could not have departed sufficiently from 293K to affect the results of this study. However the effect has been assessed by performing a sensitivity study.

(ii) Acrylic Plates

Acrylic plates were used in the experiments as the supporting structure for the fuel clusters at three positions. The upper plates are grid plates of thickness 1.27cm, and are located in the vicinity of the bottom and top of the fuel elements; however the exact positions of the plates are not given in the experimental report. The lower plate is a solid support plate of thickness 2.54cm and is located on top of the aluminium plinth.

The composition of the acrylic material is not provided, and the experimentalists argue that the plates can be accurately represented as water due to its almost identical moderating characteristics; it should be noted that the plates constitute a small proportion of the total volume of moderator. Based on this recommendation the upper acrylic plates have been replaced by water in the MONK model, due to the uncertainty about their position. However as the position of the lower plate is known, it has been modelled assuming a typical acrylic atomic composition (see Table 5.3.2). The effect of omitting the upper acrylic plates has been assessed by performing a sensitivity study.

(iii) Aluminium Rods

Aluminium spacer/support rods 1.27cm diameter and 83.9cm long were positioned at each corner of the fuel clusters, although the exact locations are not given in the experimental report. Measurements made by the experimentalists demonstrated that the aluminium safety and control guide blades had no impact on the critical separation measurements. As these are of larger volume than the aluminium rods and are closer to the fuel rod clusters, it can be concluded that the aluminium rods would also have no effect. Therefore the aluminium rods have been omitted from the MONK model and replaced by water.

(iv) Aluminium Plates

Aluminium 'L' shaped plates 5.08cm x 5.08cm x 0.635cm were positioned at the top-end of the fuel elements to provide further support for the fuel clusters; their exact positions are not given in the experimental report. An experimental sensitivity study, where the quantity of aluminium was doubled, demonstrated that the support plates did not effect the critical separation measurements. Therefore these plates have been omitted from the MONK model and replaced by water.

(v) Water

H_2O with a density 0.9982g/cm^3 [8] has been employed in the MONK model. As stated above the effect of density changes arising from temperature changes has been assessed by performing a sensitivity study. All measured trace elements have been included in the water specification employed in the MONK model. The uncertainties quoted on the trace element concentrations have been ignored as the quantities involved are negligibly small.

(vi) Absorbing Plates

The dimensions of the absorbing plates are given in the experimental report but their axial positions are not, although it is stated that the plates were slightly longer and wider than the rod clusters (note that the boral plates and the steel plates are slightly different in width). Based on this information the plates have been modelled to extend beyond the fuel length and fuel cluster width equally in each direction. The difference between this and any alternative location that met the description given in the experimental report would be negligible. The composition of the plates was taken from the experimental report. (Note - for the boral plates, the element Zn is not present in the MONK continuous energy nuclear data library. However as its weight fraction is very small it has been replaced by Al27, in keeping with common experiment modelling practice [9]).

(vii) Steel Tank

The composition of the carbon-steel tank is not given in the experimental report. It has been modelled as iron even though the experimentalists demonstrated that materials outside the reflector have negligible effect on the measured critical separation distances.

(viii) Safety and Control Components

The safety and control mechanisms are depicted in the experimental report to have been located in air above the water. The safety and control blades are fully withdrawn during measurements, presumably in the air above the water. It is therefore concluded that the safety and control mechanisms and blades are sufficiently well separated from the fuel rod clusters by the water to have a negligible effect on the critical separation measurements - they have therefore been omitted from the MONK model. The safety and control blade guides are made of aluminium and are permanently in place in the water between the fuel rod clusters. Experiments were performed where the aluminium thickness was doubled and these demonstrated no impact on the critical separation measurements. The safety and control blade guides have therefore also been omitted from the MONK model and replaced by water.

(ix) Additional Uncertainties

In addition to the sensitivity calculations mentioned above, calculations have also been performed to consider the following uncertainties in the MONK model: U235 enrichment, pin pitch, fuel clad outer diameter, fuel diameter, fuel density, and uranium isotopic composition. These are considered to provide the most significant uncertainty on the system multiplication [9].

Uncertainties on the critical separation distances and absorbing plate thicknesses are provided in the experimental report and sensitivity calculations have also been performed to assess these. It has been assumed that the quoted uncertainties on these dimensions are simply measurement uncertainties and include no allowance for any other uncertainty.

Figures 5.3.1,5.3.2 and 5.3.3 show views of the MONK model geometry and present the important dimensions. The materials used in the MONK model are presented in Table 5.3.2. Each calculation employed 1000 neutrons per stage and was run to achieve a precision of smaller than 0.0015. This ensured that adequate statistical sampling was performed, which was verified by performing detailed checking of the output. The input specification and output for each calculation were independently checked. The results from two calculations using different random number seeds were averaged for each experiment to give a combined statistical precision of 0.0010.

5.3.3 Results

(a) Standard Calculations

MONKDEV calculations have been performed as described above using the values of the critical separation distances G and X and the plate thicknesses T given in Table 5.3.1. The results obtained from the calculations are summarised in Table 5.3.3.

The calculations indicate that the Monte Carlo code MONKDEV predicts the critical system multiplication for low-enriched UO_2 fuel pins with water moderator and reflector, and with boral, steel and boron-steel absorber plates, within 0.35% of unity; a similar result is observed for the system without absorber plates. However an analysis of the experimental uncertainties is required to assess the significance of this indication of accuracy - this is considered below.

The mean calculated k-effective for the eight selected experiments is 0.9993 with a standard error of 0.0004. For the 16 MONKDEV runs, the observed external standard deviation is 0.0018 ± 0.0005 which is in good agreement with the estimated internal standard deviation of about 0.0015. This is a good check that 1000 superhistories per stage is adequate for settling to be established below the random noise level. There is no significant evidence of added statistical noise, despite the fact that the MONKDEV calculations represent eight different configurations. This suggests that the experimental measurements are of high quality and there is little or no drift in the MONKDEV bias between the configurations.

(b) Sensitivity Analysis

The effects of the various uncertainties have been examined to assess whether the above indication of the accuracy of the code is sustainable. Both the calculation and the experiment have residual errors/uncertainties that might affect the calculated value of k-effective. It is considered that the MONK model has been constructed with sufficient accuracy and the Monte Carlo sampling is adequate; therefore any deviations between the calculated and measured results are due either to errors/uncertainties in the nuclear data library used in the calculations or errors/uncertainties in the experiments.

Starting with the experimental uncertainties, these must be assessed by sensitivity analysis. The items chosen for study are those that arise from assumptions made in interpreting the experiments, from uncertainties measured by the experimentalists or from assumed uncertainties arising from the quoted precision of significant parameters.

The first stage of the sensitivity analysis consisted of performing additional MONK calculations in order to assess the sensitivity of the system multiplication to the uncertainties in

the separation distances X and G and the plate thickness T quoted in the experimental report. The unpoisoned system, one boron-steel poisoned system and the boral-poisoned system were selected for this sensitivity study.

Consequently experiments 3.01, 3.05 and 3.08 have been modified to provide the input for independent sensitivity calculations, each considering ten standard deviation increases in the relevant parameters (i.e. T+10σ, G+10σ and X+10σ). Note that for the boral-poisoned system, the increased thickness calculation considered a change in the boral only with the thickness of the aluminium coating remaining the same. The results from these calculations have then been divided by ten to estimate the change in reactivity resulting from a one standard deviation increase; the linear relationship assumed is considered sufficiently accurate for the purpose.

In addition a calculation was performed to evaluate the effect of the uncertainty in the boron composition of the plates for the case with the largest relative uncertainty (304L steel with 1.05% boron). Consequently experiment 3.04 has been modified to provide the input for a sensitivity calculation considering a five standard deviation decrease in boron content (note that for this uncertainty a ten standard deviation decrease would have resulted in too large an absolute change in boron content, making the linear scaling invalid).

The results for these calculations are summarised in Table 5.3.4, where it can be seen that the predicted reactivity changes are not significant compared with their calculated uncertainties. However in order to accommodate the statistical uncertainty in the MONK sensitivity calculations, a one standard deviation experimental uncertainty of 0.0003 (0.03%) will be assigned to cover the effect of the uncertainties on the parameters considered in this part of the sensitivity study.

The second stage of the sensitivity analysis consisted of calculations to investigate the effect of the uncertainties on various other parameters that may make a significant contribution to the total experimental uncertainty. The selection of the parameters to investigate is based on the findings of the analysis of similar experiments performed in the DIMPLE reactor at Winfrith [9]. The calculations have been performed using the LWRWIMS code [10] for the case with no poison plates and with infinite length fuel pins, and the results obtained have been used to provide an estimate of the total experimental uncertainty for the whole range of configurations. The results for the parameters that have been studied are shown in Table 5.3.5.

Note that the uncertainties ascribed to the U235 enrichment, the cladding outer diameter, the fuel outer diameter and the uranium composition have been taken from the experimental documentation. For the temperature uncertainty a maximum difference of 5K has been assumed, together with the associated material density changes. For the acrylic plate a three standard deviation estimate of the effect of displacing water has been considered which has then been scaled to produce a one standard deviation uncertainty on the basis of a linear relationship. The results when added quadratically provide an upper bound of the experimental uncertainty at the one standard deviation level of 0.0017 (0.17%) for this part of the sensitivy analysis.

Summing the uncertainties from both parts of the sensitivity analysis quadratically provides an upper bound to the total experimental one standard deviation uncertainty of 0.0017 (0.17%).

Turning to the calculated uncertainties it should be noted that MONK assumes that all fission neutrons are born in the prompt neutron energy spectrum. It has been shown [11] that for low-enriched fuel clusters separated by absorbing plates, the importance of delayed neutrons is negligible and the MONK assumption leads to a very small under-prediction in k-effective of less than 0.0001 (0.01%). The largest correction is for the case without absorber plates (3.01) for which the assumption causes an under-prediction of 0.06%. The effect is therefore always much less than the uncertainty of the MONK calculation and would lead to a correction of about 0.01% on the mean value of k-effective for the eight cases. This is considered trivial compared with the experimental and calculational uncertainties.

The experimental measurement of k-effective = 1.0000±0.0017 can therefore be compared with the calculated mean value of 0.9993±0.0004. Thus the difference between experiment and calculation is not significant even at the one standard deviation level.

(c) Comparison with MONK6B

Table 5.5.6 gives a comparison of the results for the eight experiments for the JEF2.2 library used with MONKDEV as reported above and for the current standard UKNDL-based library used with MONK6B.

As reported above the mean value for the JEF2.2 library calculations is 0.9993±0.0004. The mean value for the UKNDL calculations is 1.0034±0.0006. The differences between the two libraries is significant at the three standard deviation level, with the JEF-based library apparently providing better agreement with the experimental measurements. In each case the JEF2.2/MONKDEV result is closer to the experimental result than the UKNDL/MONK6B result. However the difference between the UKNDL calculations and experiment is not significant at the three standard deviation level.

5.3.4 Summary

This report has shown that the Monte Carlo code MONK6B calculates the average system multiplication for a series of critical experiments using low-enriched UO_2 fuel pins with water moderator and reflector, and with boral, steel and boron-steel absorber plates, within -0.07%±0.04% of unity. Correcting for the relative importance of delayed neutrons does not significantly alter this result. The calculated deviation from unity compares with an estimated total experimental error of 0.17% (assumed 1σ). Thus the apparent small negative bias on the mean calculated value is not statistically significant even at the one standard deviation level and could be due solely to a combination of experimental and calculational uncertainties.

Table 5.3.1 - MEASURED CRITICAL SEPARATION DISTANCES

Case No.	Absorber Material	Absorber Plate Thickness (T) cm	Distance between Plates and Fuel (G) cm	Fuel Cluster Separation Distance (X) cm
3.01	None	-	-	10.64 ± 0.01
3.02	304L Steel (no boron)	0.302 ± 0.013	0.428 ± 0.032	9.22 ± 0.01
3.03	304L Steel (no boron)	0.302 ± 0.013	3.277 ± 0.032	9.76 ± 0.03
3.04	304L Steel (1.05% boron)	0.298 ± 0.006	0.432 ± 0.030	6.10 ± 0.01
3.05	304L Steel (1.05% boron)	0.298 ± 0.006	3.277 ± 0.032	8.08 ± 0.02
3.06	304L Steel (1.62% boron)	0.298 ± 0.005	0.432 ± 0.030	5.76 ± 0.02
3.07	304L Steel (1.62% boron)	0.298 ± 0.005	3.277 ± 0.032	7.90 ± 0.03
3.08	Boral	0.713 ± 0.011 *	3.277 ± 0.032	6.72 ± 0.01

* includes 0.102cm Aluminium coating on each surface

Table 5.3.2 - SUMMARY OF MATERIAL DATA

Material	Density g/cm³	Nuclides Present	Fractions by Atom or Weight
UO_2 - 4.306% enriched-by-weight (1) (by weight)	10.4	U234 U235 U236 U238 O	1.9400E-4 3.7917E-2 1.9400E-4 8.4225E-1 1.1945E-1
Rubber end caps (by weight)	1.321	C HinH2O Ca S32 O Si	5.8000E-1 6.5000E-2 1.1400E-1 1.7000E-2 2.2100E-1 3.0000E-3
Aluminium (by weight)	2.692	Al27 (2) Cr Cu Fe Mn Si Ti S32 (3)	9.7150E-01 2.1000E-03 1.2000E-03 8.2000E-03 2.1000E-03 8.2000E-03 6.1000E-03 6.0000E-04
Water (by weight)	0.9982 (4)	HinH2O O Cl N Al27 (2) F19 (5) Cd S32 (3)	1.1188E-01 8.8809E-01 3.0000E-05 9.5000E-08 2.6000E-07 1.5000E-07 6.0100E-09 2.6400E-06
Acrylic (6) (by atom)	1.18	HinH2O (7) O C	8.00000E+00 2.00000E+00 5.00000E+00
Iron (by weight)	7.86	Fe	1.00000E+00

Table 5.3.2 - SUMMARY OF MATERIAL DATA (continued)

Material	Density g/cm³	Nuclides Present	Fractions by Atom or Weight
Boral (by weight)	2.49	Al27 (2) (10)	6.2490E-01
		B10 (8)	5.2900E-02
		B11	2.3410E-01
		C	7.9700E-02
		Cr	5.0000E-04
		Cu	9.0000E-04
		Fe	3.3000E-03
		Mg	5.0000E-04
		Mn	5.0000E-04
		Ni	2.0000E-04
		Si	2.0000E-03
		Na23 (9)	2.0000E-04
		S32 (3)	3.0000E-04
304L Steel (no boron) (by weight)	7.930	Cr	1.8560E-01
		Cu	2.7000E-03
		Fe	6.8240E-01
		Mn	1.5800E-02
		Mo	2.6000E-03
		Ni	1.1090E-01
304L Steel (1.05% boron) (by weight)	7.900	Cr	1.9030E-01
		Cu	2.8000E-03
		Fe	6.8040E-01
		Mn	1.5800E-02
		Mo	4.9000E-03
		Ni	9.5300E-02
		B10 (8)	1.9350E-03
		B11	8.5650E-03
304L Steel (1.62% boron) (by weight)	7.770	Cr	1.9600E-01
		Cu	2.6000E-03
		Fe	6.6400E-01
		Mn	1.6900E-02
		Mo	3.1000E-03
		Ni	1.0120E-01
		B10 (8)	2.9860E-03
		B11	1.3214E-02

Notes on Table 5.3.2

(1) The experimental report [5] quotes the fuel enrichment as 4.29 wt% U235 enriched UO_2 rods. However this figure was re-evaluated in 1980 to 4.31 wt%.

(2) The MONK nuclide is Al27 which has a natural abundance of 100% [8].

(3) The MONK nuclide is S32 which has a natural abundance of 95% [8] - the difference is negligible at the low concentration present.

(4) Density of water is taken from Reference 8.

(5) The MONK nuclide is F19 which has a natural abundance of 100% [8].

(6) Acrylic composition taken from experimental documentation.

(7) The MONK nuclide HinH2O is recommended for all occurrences of bound hydrogen [1].

(8) The boron composition is taken from Reference 8.

(9) The MONK nuclide is Na23 which has a natural abundance of 100% [8].

(10) Zinc is not present in the MONK nuclear data library. In very low concentrations it can be accurately modelled as aluminium [9]. The aluminium weight fraction used here includes the Zinc weight fraction given in the experimental report.

Table 5.3.3 - RESULTS FROM STANDARD MONK CALCULATIONS

Case No.	Absorber Material	k-effective - run 1	k-effective - run 2	Mean k-effective
3.01	None	1.0006 (0.0014)	0.9976 (0.0015)	0.9992 (0.0011)
3.02	304L Steel (no boron)	0.9957 (0.0015)	0.9972 (0.0015)	0.9965 (0.0011)
3.03	304L Steel (no boron)	0.9999 (0.0015)	0.9986 (0.0015)	0.9993 (0.0011)
3.04	304L Steel (1.05% boron)	0.9996 (0.0015)	0.9987 (0.0015)	0.9992 (0.0011)
3.05	304L Steel (1.05% boron)	1.0015 (0.0015)	0.9981 (0.0015)	0.9998 (0.0011)
3.06	304L Steel (1.62% boron)	1.0022 (0.0015)	0.9969 (0.0015)	0.9996 (0.0011)
3.07	304L Steel (1.62% boron)	0.9998 (0.0015)	0.9999 (0.0015)	0.9999 (0.0011)
3.08	Boral	1.0009 (0.0014)	1.0009 (0.0015)	1.0009 (0.0010)

The figure in brackets for the individual calculations is the standard deviation estimated by MONK. For the mean value the figure in brackets is the standard error on the mean value computed using the standard deviations from the two independent calculations.

Table 5.3.4 - RESULTS FROM MONK SENSITIVITY CALCULATIONS

Case No.	parameter uncertainty	k-effective	uncertainty in k-effective (Δk) from 1σ change
3.01		1.0038 (0.0011)	
3.01A	X+10σ	1.0063 (0.0010)	0.0003 (0.0001)
3.05		1.0015 (0.0011)	
3.05A	T+10σ	1.0041 (0.0011)	0.0003 (0.0001)
3.05B	G+10σ	1.0023 (0.0011)	0.0001 (0.0001)
3.05C	X+10σ	1.0034 (0.0011)	0.0002 (0.0001)
3.08		1.0032 (0.0010)	
3.08A	T+10σ	1.0030 (0.0010)	0.0000 (0.0001)
3.08B	G+10σ	1.0039 (0.0011)	0.0001 (0.0001)
3.08C	X+10σ	1.0035 (0.0011)	0.0000 (0.0001)
3.04		1.0045 (0.0011)	
3.04A	5σ reduction in boron content	1.0052 (0.0010)	0.0001 (0.0001)

The figure in brackets in the mean k-effective column is the standard error on the mean value computed using the standard deviations from two independent calculations. The difference is computed by subtracting the reference case multiplication and scaling. The resulting standard error is given in brackets.

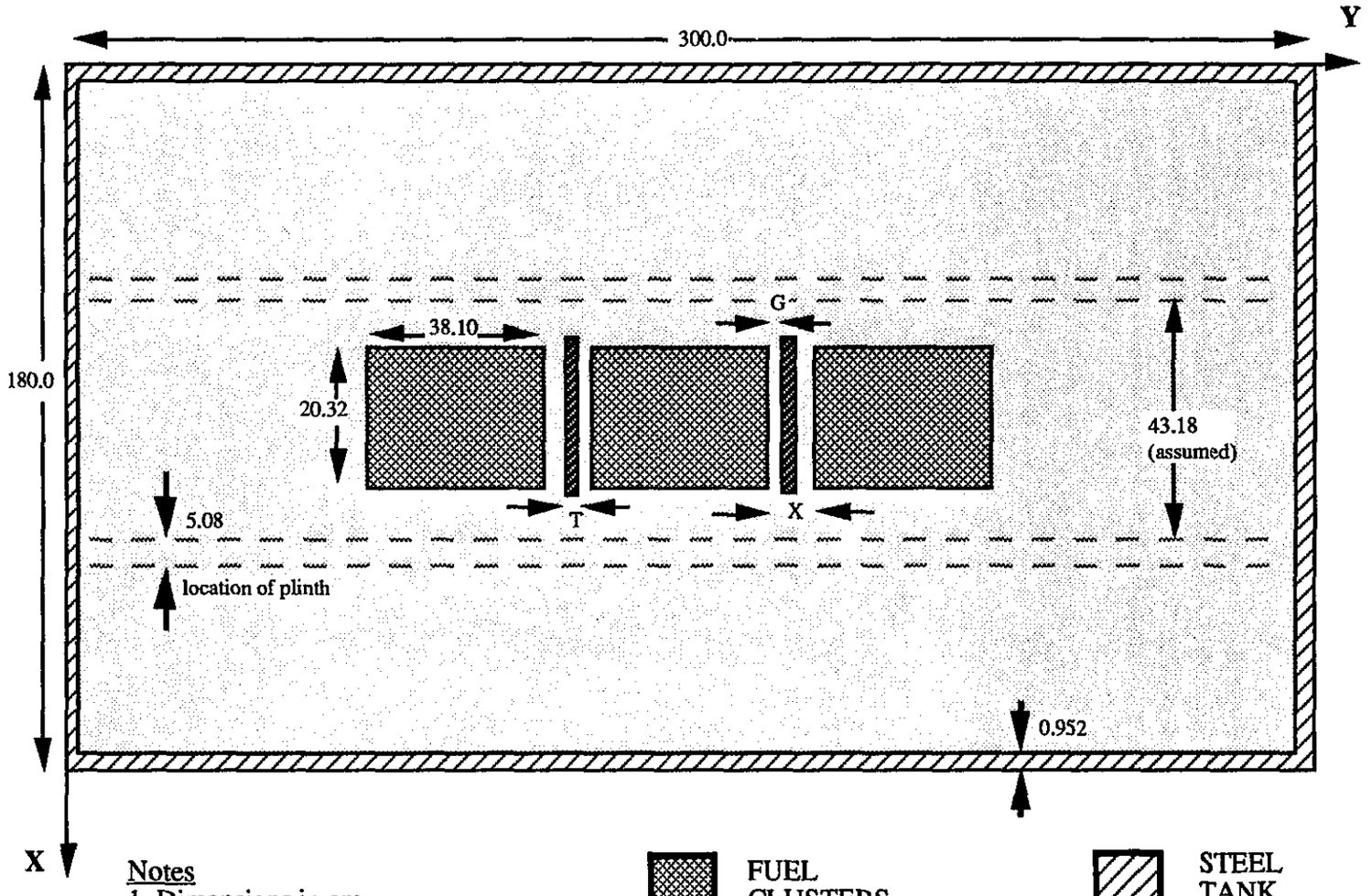
Table 5.3.5 - RESULTS FROM LWRWIMS SENSITIVITY CALCULATIONS

Parameter	parameter uncertainty (1σ assumed unless stated)	LWRWIMS-predicted 1σ uncertainty in k-effective (Δk)
U235 enrichment	0.013%	0.00060
Pin pitch (random uncertainty in last significant figure)	0.005cm	0.00050
Cladding outer diameter	0.003cm	0.00037
Fuel outer diameter	0.003cm	0.00077
Temperature	5K	0.00044
UO_2 density	0.06g/cm^3	0.00084
Acrylic plates (acrylic comprising 3% of moderator volume - assumed 3σ uncertainty)	displacement of water	0.00089

Table 5.3.6 - COMPARISON WITH MONK6B

Case No.	Mean k-effective - JEF2.2/MONKDEV	Mean k-effective - UKNDL/MONK6B
3.01	0.9992 (0.0011)	1.0038 (0.0011)
3.02	0.9965 (0.0011)	1.0032 (0.0011)
3.03	0.9993 (0.0011)	1.0063 (0.0011)
3.04	0.9992 (0.0011)	1.0045 (0.0011)
3.05	0.9998 (0.0011)	1.0015 (0.0011)
3.06	0.9996 (0.0011)	1.0033 (0.0011)
3.07	0.9999 (0.0011)	1.0015 (0.0011)
3.08	1.0009 (0.0010)	1.0032 (0.0010)

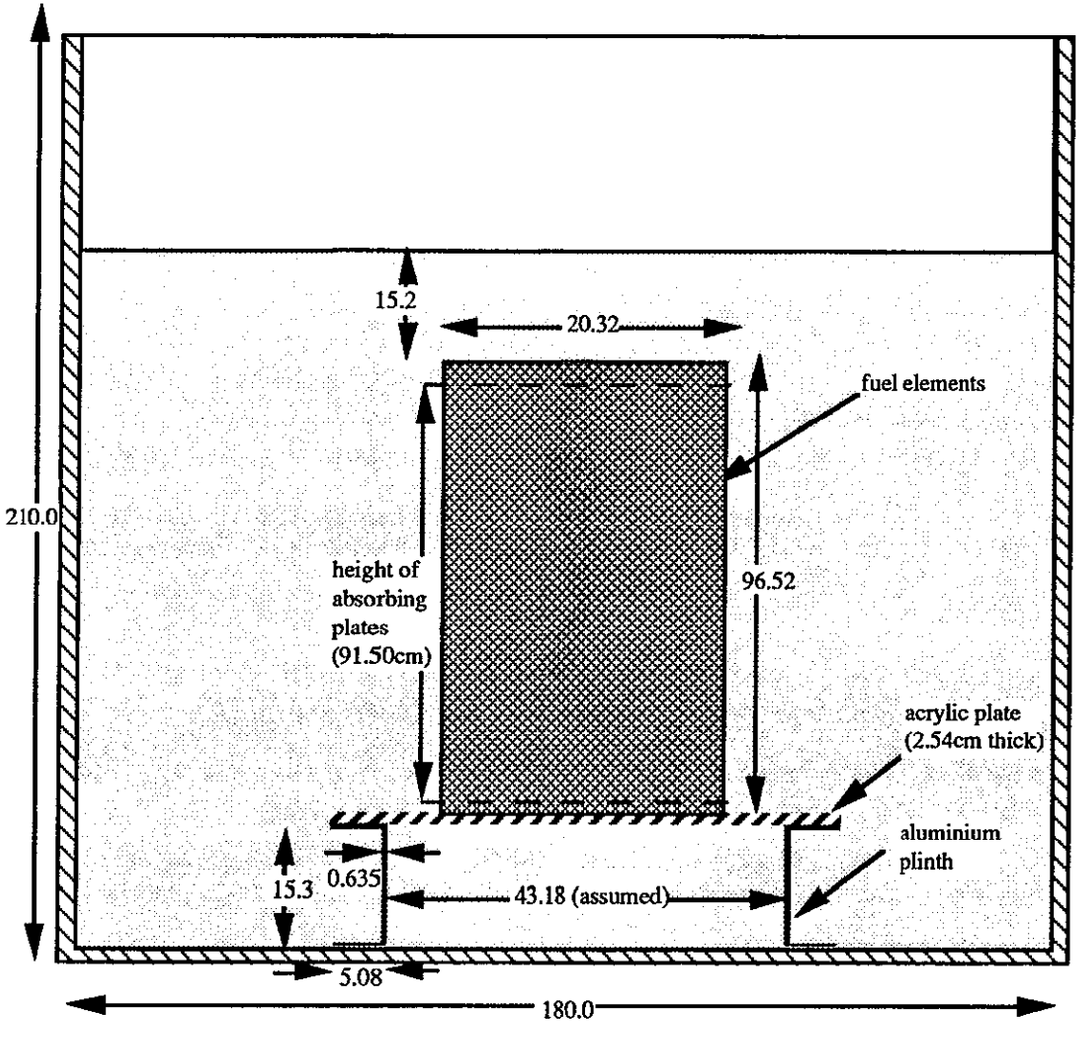
The figure in brackets is the standard error estimated by MONK.



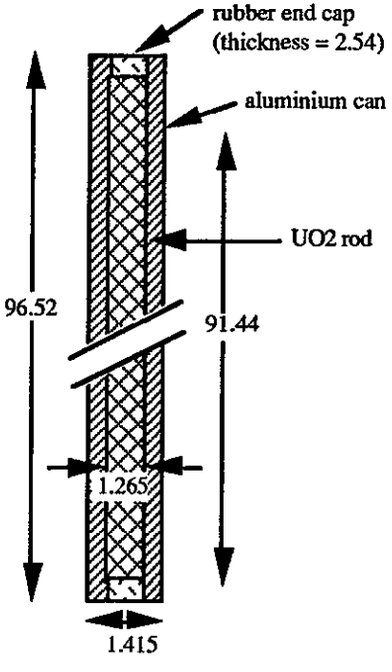
Notes
1. Dimensions in cm
2. Drawing not to scale
3. Dimensions T,G, and X are given in Table 1, and are shown more clearly in Figure 5.3.3

FUEL CLUSTERS
BORAL PLATES
STEEL TANK
WATER

Figure 5.3.1 - PLAN VIEW OF THE MONK MODEL



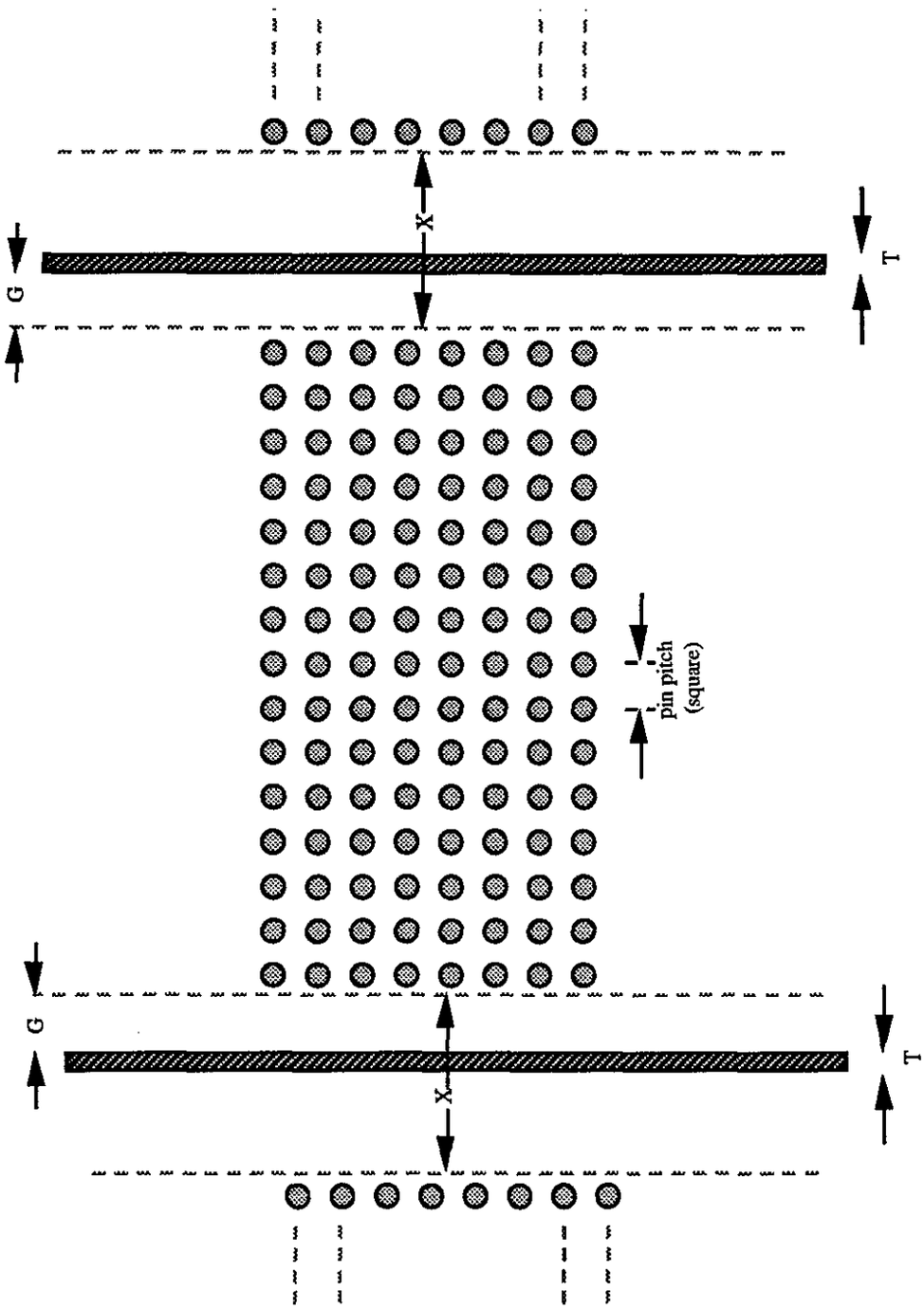
ENLARGED VIEW OF FUEL ELEMENT



Notes
1.Dimensions in cm
2.Drawing not to scale

Figure 5.3.2 - SECTIONAL VIEW OF THE MONK MODEL

Figure 5.3.3 - DETAILED PLAN VIEW OF THE CENTRAL FUEL CLUSTER



Notes
1. Drawing not to scale
2. See Figure 5.3.1 for overall plan view

5.4 Experiment Number 4

5.4.1 Experimental Description

The experimental programme from which the experiments were selected was performed at the Battelle PNL Critical Mass Laboratory [6] during the 1960's.

The experimental programme considered rectangular parallelepipeds of homogeneous PuO_2/polystyrene with and without a Plexiglas reflector. Various Pu240 contents and H:Pu atom ratios were employed. The aim of the programme was to determine criticality parameters of plutonium mixtures having concentrations that are typical of wet powders, precipitates, slurries and polymers. This study concentrates on fuel with 11.5 wt% Pu240 enriched PuO_2/polystyrene and a 5 H:Pu atom ratio.

The experimental configuration comprised an array of rectangular PuO_2/polystyrene blocks stacked on a remote split-table machine. The blocks were fabricated by compacting polystyrene and PuO_2 into rectangular parallelepiped moulds. Most blocks were 5.12 x 5.12 x 3.81cm although blocks of smaller height were produced to facilitate the construction of critical arrays. Each compacted block was sprayed with a thin coat of aluminium paint (~0.0025cm) and covered with rubberised plastic (~0.02cm).

The experiments consisted of assembling different sized arrays of the compacted blocks to form critical configurations. The experimental method comprised source-neutron multiplication measurements for successive block additions during the assembly of the critical arrays. Spontaneous fission, primarily from Pu240, supplied the required neutron source. Three proportional neutron counters provided measurements of the source multiplication.

Although each experimental configuration was made critical, the point of criticality was usually achieved with an incomplete top layer of blocks and with a control rod partially inserted. A least-squares analysis was used to convert these measurements into the clean critical dimensions given in the experimental report [6]. These critical dimensions were also corrected by the experimentalists for:

- stacking voids, cladding and reflection from the table for the bare assembly
- stacking voids and cladding in the reflected assemblies (note that the 15cm reflector isolates the assembly from the table top for the reflected cases)

The critical dimensions used in the validation study are given in Table 5.4.1. The five experiments are given case numbers 4.01 to 4.05 respectively.

5.4.2 The MONK Model

The MONK models of the experiments have been constructed from the data presented in Reference 6. However, it is important to note the following differences between the experimental conditions and the models used in the calculations:

(i) Temperature Effects

Standard room temperature modelling at 293K has been employed for Doppler broadening all reaction cross-sections. The actual temperature distribution of the experimental apparatus is recorded as 333K±10K. The effect of this temperature difference has been assessed by employing handbook data.

(ii) Cladding

The critical dimensions quoted in the experimental report have been corrected by the experimentalists for stacking voids and cladding. These corrections were designed to produce clean experimentally derived data for unclad close-fitting blocks (i.e. a homogeneous region of PuO_2/polystyrene). A sensitivity study has been carried out to assess the magnitude of the uncertainty in this correction.

(iii) Table Top and Structural Supports

As stated earlier the critical dimensions in the bare case have been corrected to account for the reflection from the aluminium table top. A sensitivity study has been carried out to assess the magnitude of the uncertainty in this correction.

(iv) Additional Uncertainties

In addition to the sensitivity studies mentioned above, calculations have been performed to consider the following uncertainties in the MONK model: critical height, plutonium isotopic composition, H:Pu atom ratio.

Figure 5.4.1 shows a view of the MONK model geometry for a reflected case and presents the important dimensions. The materials used in the MONK model are presented in Table 5.4.2. Each calculation employed 1000 neutrons per stage and was run to achieve a precision of smaller than 0.0015. This ensured that adequate statistical sampling was performed, which was verified by performing detailed checking of the output. The input and output data for each calculation were independently checked. The results from two calculations using different random number seeds were averaged for each experiment to give a combined statistical precision of about 0.0010 (0.1%).

5.4.3 Results

(a) Standard Calculations

MONKDEV calculations have been performed as described above using the critical dimensions given in Table 5.4.1. The results obtained from the calculations are summarised in Table 5.4.3.

The calculations show that the Monte Carlo code MONKDEV over-predicts the system multiplication for the five cases by between 0.9% and 1.3%. However an analysis of the experimental uncertainties and corrections is required to see whether this over-prediction is significant. This is considered in the next section.

The mean value of k-effective for the four reflected experiments is 1.0120 with a standard error of 0.0004. In the eight reflected MONKDEV runs, the observed external standard deviation is 0.0015±0.0004 which is not significantly different from the internal standard deviation of 0.0015. This is a good check that 1000 neutrons per stage is adequate for settling to be established below the random noise level. There is no significant evidence of added statistical noise, despite the fact that the MONKDEV calculations represent four different configurations. This suggests that the experimental measurements are of a reasonable quality and there is no drift in the MONKDEV bias between the configurations.

Additional calculations were performed using thermal scattering data for hydrogen in polythene rather than hydrogen in water for the polystyrene and Plexiglas. The results are given Table 5.4.3 and show that the change in data does not significantly affect the calculated values of k-effective.

(b) Sensitivity Analysis

The effects of the various uncertainties have been examined to assess whether the above indication of the accuracy of the code is sustainable. Both the calculations and the experiments have residual errors/uncertainties that might effect the value of k-effective. It is considered that the experimental geometry has been modelled with sufficient accuracy and the Monte Carlo sampling is adequate; therefore any deviations between the calculated and measured results are due either to errors/uncertainties in the nuclear data library used in the calculations or errors/uncertainties in the experiments. The experimental report quotes random reproducibility uncertainties but the systematic uncertainties must be assessed in a sensitivity analysis.

An uncertainty is introduced into the nuclear data used in the calculations due the temperature of the experiments. The temperature quoted in the experimental report at each core centre is 333±10K equating to a 40K difference between the calculation temperature and the experimental situation. The Manual of Criticality Data [12] contains information on a similar type of fuel [homogeneous $Pu(2.2)O_2$/polystyrene at 15 H:Pu atom ratio] at similar core temperatures. Reactivity worths of -3cents/K for unreflected cases and -0.25cents/K for reflected cases are quoted. Using a delayed neutron fraction for Pu239 in a fast spectrum of 0.0020 [13], these convert to -6mN/K for unreflected cases and -0.5mN/K for reflected cases. Therefore a correction of the order of -0.0024 (0.24%) should be applied to the unreflected result and -0.0002 (0.02%) to the reflected results.

The first stage of the sensitivity analysis of the experiment consisted of performing additional MONK calculations in order to assess the sensitivity of the system multiplication to the following quoted uncertainties: critical height, Pu239 content, Pu240 content, H:Pu atom ratio. Note that the Pu239 and Pu240 content uncertainties are not independent as the residue of the total plutonium content is made up with the other nuclide in each case. Therefore, only the largest of the two values has been included in the total uncertainty. Changes in the absolute level of plutonium are considered in the uncertainty in H:Pu atom ratio.

The sensitivity calculations were performed with the unreflected case and one reflected case assumed to be representative of all the reflected configurations. Consequently experiments 4.01 and 4.03 have been modified to provide the input for independent sensitivity calculations considering ten standard deviation increases in relevant parameters. The equivalent change in multiplication for a one standard deviation increase has been computed by assuming a linear relationship. For the unreflected case the reflection from the remote split-table has been considered by incorporating a representation of the table in a further calculation. The results of these calculations are given in Table 5.4.4 which shows that the total uncertainty at the one standard deviation level from this part of the sensitivity analysis is ±0.0030 (0.30%) for the unreflected assembly and ±0.0016 (0.16%) for the reflected assemblies.

The second stage of the sensitvity analysis consisted of assessing the uncertainties associated with the corrections made by the experimentalists in deriving the clean critical dimensions given in the experimental report. Firstly additional calculations have been performed to assess the effect of the uncertainties associated with the stacking and void corrections. In order to analyse these effects a hypothetical case (not a quoted critical configuration) has been employed comprising an array of whole blocks (6x6x4).

The stacking and void corrections made by the experimentalists were determined by evaluating the effect of multiple layers of cladding and void thickness and extrapolating back to zero in each case based on linear relationship assumptions. This has been simulated here for the hypothetical case 4.S1 and the results are summarised in Table 5.4.5.

The results from cases 4.S1 and 4.S1A show a combined reactivity change of 0.0074±0.0016 for the clad and the void thickness. The reactivity change due to the clad alone is obtained by comparing cases 4.S1A and 4.S1B and results in a value of 0.0033±0.0015. Similarly, from cases 4.S1A and 4.S1C the void alone is worth 0.0039±0.0016. The effect of clad and void have the same sign (both reducing reactivity) and within the calculated uncertainties combine to give the calculated joint reactivity change. Within the calculated uncertainties, this provides confidence in the accuracy of the experimental corrections.

Based on the results of cases 4.03, 4.S1 and 4.S1A, the resulting correction needed to account for the stacking voids and cladding is of the order of 0.46±0.16cm. This is consistent with the correction of 0.59cm observed in the experimental documentation. Therefore it is considered prudent to include an additional one standard deviation uncertainty on the critical height of 0.16cm which, based on the results of the first stage of the sensitivity analysis, equates to an additional multiplication uncertainty of 0.0011 for the unreflected case and 0.0016 for the reflected cases.

The other significant correction made by the experimentalists was the conversion of incomplete top layers of blocks and control rod insertion levels into corresponding clean dimensions. No assessment of the uncertainty in this correction is given in the experimental reports but it seems reasonable to assign a similar level of uncertainty as used in the clad and void analysis. This leads therefore to a further experimental uncertainty of 0.0011 for the unreflected case and 0.0016 for the reflected case. Hence the total experimental uncertainty from the second stage of the sensitivity analysis is ±0.0016 (0.16%) for the unreflected case and ±0.0023 (0.23%) for the reflected cases.

Combining the results of the two parts of the sensitivity analysis provides an estimate of the total experimental uncertainty at the one standard deviation level of 0.0034 for the unreflected case and 0.0028 for the reflected cases.

(c) Comparison with MONK6B

Table 5.4.6 gives a comparison of the results for the five experiments for the JEF2.2 library used with MONKDEV as reported above and for the current standard UKNDL-based library used with MONK6B.

As reported above the mean value for the JEF2.2 library reflected calculations is 1.0120±0.0004. The mean value for the UKNDL calculations is 1.0186±0.0014. The differences between the two libraries is significant at the three standard deviation level, with the JEF-based library apparently providing better agreement with the experimental measurements. In each case the JEF2.2/MONKDEV result is closer to the experimental result than the UKNDL/MONK6B result. For the unreflected case the difference between the two calculations is even more marked with a 2% reduction in k-effective. The spectrum for the unreflected case is very different than that for the reflected cases, with the reduction in k-effective arising largely from a significant reduction in Pu239 fission within the intermediate/fast energy range.

5.4.4 Summary

This report has shown that the Monte Carlo code MONKDEV over-predicts the average system multiplication for a series of critical experiments using Plexiglas-reflected 11.5 wt% Pu240 enriched PuO_2/polystyrene blocks with a 5 H:Pu atom ratio by 1.20%±0.04%. For a similar unreflected assembly the over-prediction is 0.97%±0.11%. Correcting for the effect of temperature does not significantly effect the result for the reflected cases, but does cause a 0.24% (approximate) reduction in the calculated k-effective for the unreflected case.

The calculated deviation from unity compares with an estimated total experimental uncertainty of ±0.28% (1σ) for the reflected assemblies and ±0.34% (1σ) for the unreflected assembly. Thus the apparent positive bias on the mean calculated value is significant at the three standard deviation level for the reflected cases and is unlikely to be due solely to a combination of experimental and calculational uncertainties. Once the temperature correction is taken into account the result for the unreflected case is significant only at the two standard deviation level.

The experimental uncertainty arising from the corrections applied to obtain the clean critical dimensions suggest that this set of experiments does not meet the full requirements of a benchmark experiment. However this set of experiments covers an important area of application that is otherwise poorly served by experimental data and so its inclusion is justified.

Table 5.4.1 - EXPERIMENTAL CRITICAL DIMENSIONS

Case No.	Reflected with 15cm of Plexiglas	Number of Unclad Blocks		
		length (each block = 5.120cm)	width (each block = 5.120cm)	height (each block = 3.810cm)
4.01	No	7	7	7.564
4.02	Yes	5	5	4.811
4.03	Yes	6	6	3.721
4.04	Yes	8	8	2.779
4.05	Yes	10	10	2.373

Table 5.4.2 - SUMMARY OF MATERIAL DATA

Material	Density g/cm³	Nuclides Present	Fraction by weight	Atomic concentration (10^{24} atoms/cm³)
Fuel - $Pu(11.5)O_2$/polystyrene	3.241	Pu239 Pu240 Pu241 Pu242 HinH2O O C	0.6105 0.0814 0.0171 0.0013 0.0151 0.0950 0.1796	4.986E-3 6.623E-4 1.382E-4 1.026E-5 2.920E-2 1.159E-2 2.920E-2
Cladding	1.120	HinH2O C Cl	0.067 0.553 0.380	4.489E-2 3.111E-2 7.240E-3
Reflector - Plexiglas	1.185	HinH2O C O	0.08 0.60 0.32	5.666E-2 3.570E-2 1.428E-2

Table 5.4.3 - RESULTS FROM STANDARD MONK CALCULATIONS

Case No.	k-effective - run1	k-effective - run2	Mean k-effective
4.01	1.0104 (0.0015)	1.0089 (0.0015)	1.0097 (0.0011)
4.02	1.0110 (0.0015)	1.0140 (0.0015)	1.0125 (0.0011)
4.03	1.0127 (0.0015)	1.0131 (0.0015)	1.0129 (0.0011)
4.04	1.0119 (0.0015)	1.0105 (0.0015)	1.0112 (0.0011)
4.05	1.0129 (0.0015)	1.0096 (0.0015)	1.0113 (0.0011)
4.01 (1)	1.0102 (0.0014)	1.0092 (0.0015)	1.0097 (0.0010)
4.02 (2)	1.0144 (0.0015)	1.0149 (0.0015)	1.0147 (0.0011)

The figure in brackets for the individual calculations is the standard deviation estimated by MONK. For the mean value the figure in brackets is the standard error on the mean value computed using the standard deviations from the two independent calculations.

Notes on Table 5.4.3

(1) Calculation 4.01 repeated using hydrogen in polythene data in the polystyrene in place of hydrogen in water

(2) Calculation 4.01 repeated using hydrogen in polythene data in the polystyrene and Plexiglas in place of hydrogen in water

Table 5.4.4 - RESULTS FROM MONK SENSITIVITY CALCULATIONS

Case No.	Uncertainty	Mean k-effective	Difference in k-effective from 1σ change
4.01	Reference case	1.0279 (0.0011)	
4.01A	Critical height	1.0317 (0.0011)	0.0004 (0.0002)
4.01B	Pu239 content	1.0366 (0.0011)	0.0009 (0.0002)
4.01C	Pu240 content	1.0193 (0.0011)	0.0009 (0.0002)
4.01D	H:Pu atom ratio - hydrogen content	1.0560 (0.0011)	0.0028 (0.0002)
4.01E	Reflections from split-table	1.0282 (0.0011)	0.0003 (0.0016)
4.03	Reference case	1.0211 (0.0011)	
4.03A	Critical height	1.0225 (0.0011)	0.0001 (0.0002)
4.03B	Pu239 content	1.0318 (0.0011)	0.0011 (0.0002)
4.03C	Pu240 content	1.0124 (0.0011)	0.0009 (0.0002)
4.03D	H:Pu atom ratio - hydrogen content	1.0332 (0.0011)	0.0012 (0.0002)

The figure in brackets in the mean k-effective column is the standard error on the mean value computed using the standard deviations from two independent calculations. The difference is computed by subtracting the reference case multiplication and scaling. The resulting standard error is given in brackets.

Table 5.4.5-CALCULATIONS TO CHECK EXPERIMENTAL CORRECTIONS

Case No.	Uncertainty	Mean k-effective	Difference in k-effective
4.S1	Reference	1.0381 (0.0011)	
4.S1A	Clad + stacking voids	1.0307 (0.0011)	0.0074 (0.0016)
4.S1B	2xClad + stacking voids	1.0274 (0.0010)	0.0107 (0.0015)
4.S1C	Clad + 2xstacking voids	1.0268 (0.0011)	0.0113 (0.0016)

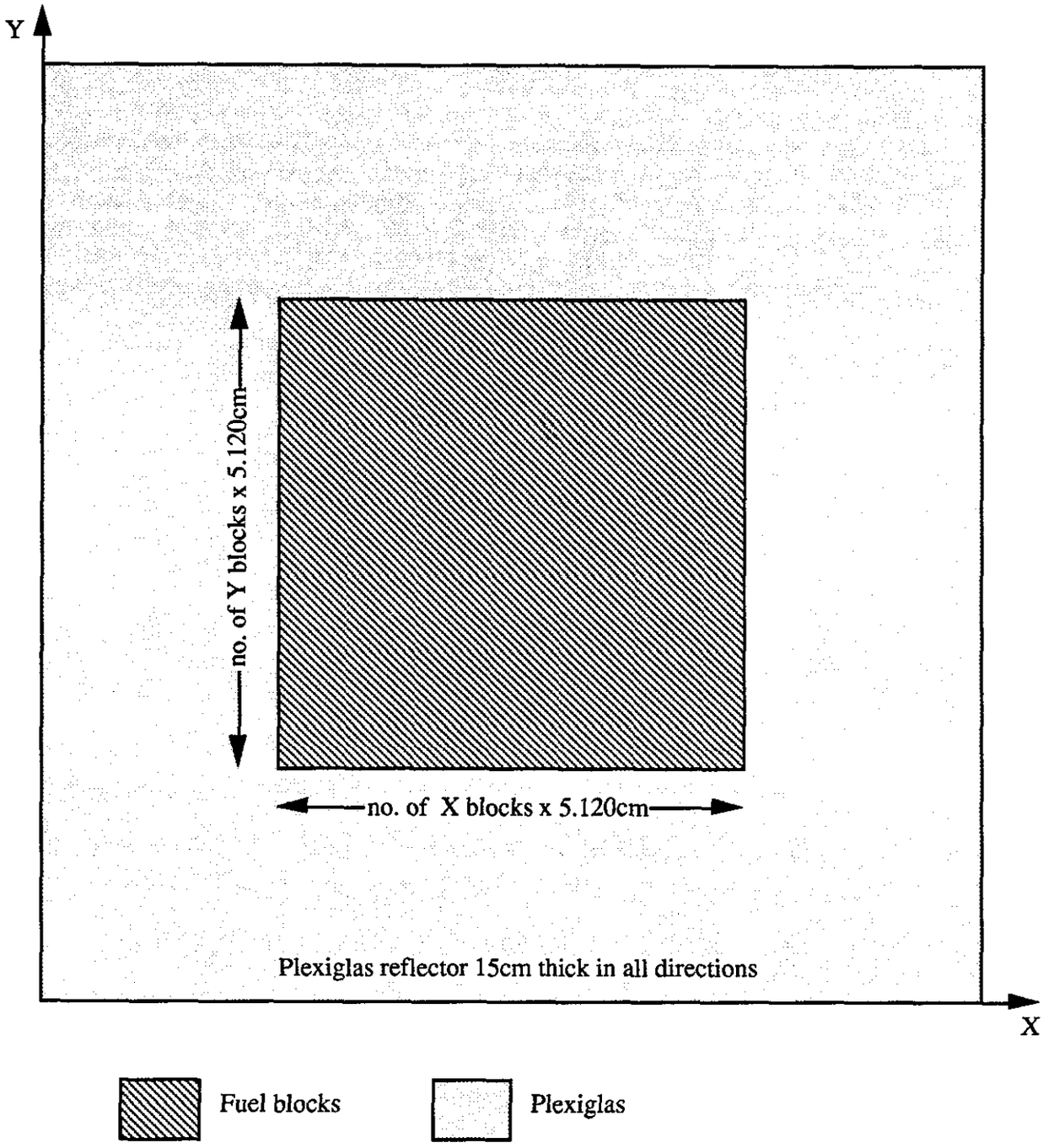
The figure in brackets in the mean k-effective column is the standard error on the mean value computed using the standard deviations from two independent calculations. The difference is computed by subtracting the reference case multiplication. The resulting standard error given in brackets.

Table 5.4.6 - COMPARISONS WITH MONK6B

Case No.	Mean k-effective - JEF2.2/MONKDEV	Mean k-effective - UKNDL/MONK6B
4.01	1.0097 (0.0011)	1.0279 (0.0011)
4.02	1.0125 (0.0011)	1.0209 (0.0011)
4.03	1.0129 (0.0011)	1.0211 (0.0011)
4.04	1.0112 (0.0011)	1.0165 (0.0010)
4.05	1.0113 (0.0011)	1.0157 (0.0011)

The figure in brackets is the standard error estimated by MONK.

Figure 5.4.1 - PLAN VIEW OF THE MONK MODEL (reflected case)



Notes
1. Drawing not to scale
2. Dimension in Z direction = no. of Z blocks x 3.810cm

5.5 Experiment Number 5

5.5.1 Experimental Description

The experimental programme from which the experiments were selected was performed at the Battelle PNL Critical Mass Laboratory [7] during the 1970's.

The experimental programme considered rectangular parallelepipeds of homogeneous PuO_2/ UO_2/ polystyrene with a Plexiglas reflector. The aim of the programme was to determine criticality parameters of mixed PuO_2/UO_2 fuels containing 30.0, 14.62 and 7.86 wt% Pu and having H:(Pu+U) atomic ratios of 47.4, 30.6 and 51.85 respectively. In all three fuels the plutonium contained 8 wt% Pu240 and the uranium was depleted to 0.151 wt% U235. This study concentrates solely on fuel with 7.86 wt% Pu present in the fuel and a 51.85 H:(Pu+U) atom ratio.

The experimental configuration comprised an array of rectangular PuO_2/ UO_2/ polystyrene blocks stacked on a remote split-table machine. The blocks were fabricated by compacting polystyrene and a homogeneous mixture of PuO_2/ UO_2 into rectangular parallelepiped moulds. Most blocks were 5.09 x 5.08 x 5.09 cm although blocks of smaller height were produced to facilitate the construction of critical arrays. Each compacted block was sprayed with a thin coat of aluminium paint (~0.0025cm) and covered with rubberised plastic (~0.02cm).

The experiments consisted of assembling different sized arrays of the compacted blocks to form critical configurations. The experimental method comprised source-neutron multiplication measurements for successive block additions during the assembly of the critical arrays. Spontaneous fission, primarily from Pu240, supplied the required neutron source. Three proportional neutron counters provided measurements of the source multiplication.

Although each experimental configuration was made critical, the point of criticality was usually achieved with an incomplete top layer of blocks and with a control rod partially inserted. A least-squares analysis was used to convert these measurements into the clean critical dimensions given in the experimental report [7]. These critical dimensions were also corrected by the experimentalists for stacking voids and cladding.

The critical dimensions used in the validation study are given in Table 5.5.1. The seven experiments are given case numbers 5.01 to 5.07 respectively.

5.5.2 The MONK Model

The MONK models of the experiments have been constructed from the data presented in Reference 7. However, it is important to note the following differences between the experimental conditions and the models used in the calculations:

(i) Temperature Effects

Standard room temperature modelling at 20 degrees C has been employed for Doppler broadening all reaction cross-sections. The actual room temperature of the experimental apparatus was 20±2 degrees C. The core centre temperature of the compacts was measured as 30±2 degrees C. The effect of this temperature difference has been assessed by employing handbook data.

(ii) Cladding

The critical dimensions quoted in the experimental report have been corrected by the experimentalists for stacking voids and cladding. These corrections were designed to produce clean experimentally derived data for unclad close-fitting blocks (i.e. a homogeneous region of PuO_2 / UO_2 / polystyrene). A sensitivity study has been carried out to assess the magnitude of the uncertainty in these corrections.

(iii) Additional Uncertainties

In addition to the sensitivity studies mentioned above, calculations have been performed to consider the following uncertainties in the MONK model: critical height, critical width and length, plutonium isotopic composition, uranium isotopic composition and the H:(Pu+U) atom ratio.

Figure 5.5.1 shows a view of the MONK geometry and presents the important dimensions. The materials used in the MONK model are presented in Table 5.5.2. Each calculation employed 1000 neutrons per stage and was run to achieve a precision of smaller than 0.0015 in k-effective. This ensured that adequate statistical sampling was performed, which was verified by performing detailed checking of the output. The input and output data for each calculation were independently checked. The results from two calculations using different random number seeds were averaged for each experiment to give a combined statistical precision of about 0.0010 (0.1%).

5.5.3 Results

(a) Standard Calculations

MONKDEV calculations have been performed as described above using the critical dimensions given in Table 5.5.1. The results obtained from the calculations are summarised in Table 5.5.3.

The calculations show that the Monte Carlo code MONKDEV over-predicts the system multiplication for the seven cases by between 2.8% and 4.1%. An analysis of the experimental uncertainties and corrections is required to see whether this over-prediction is significant. This is considered in the next section.

The mean value of k-effective for the seven experiments is 1.0323 with a standard error of 0.0019. In the fourteen MONK runs, the observed external standard deviation is 0.0048±0.0009 which is significantly greater than the internal standard deviation of 0.0015. This suggests that the experimental uncertainties are significantly greater than the statistical uncertainties of the calculations, as one would not expect a drift in the MONK bias between the different configurations.

(b) Sensitivity Analysis

The effects of the various uncertainties have been examined to assess whether the above indication of the accuracy of the code is sustainable. Both the calculations and the experiments have residual errors/uncertainties that might effect the value of k-effective. It is considered that the experimental geometry has been modelled with sufficient accuracy and the Monte Carlo sampling is adequate; therefore any deviations between the calculated and measured results are due either to errors/uncertainties in the nuclear data library used in the calculations or errors/uncertainties in the experiments. The experimental report quotes random reproducibility uncertainties but the systematic uncertainties must be assessed in a sensitivity analysis.

An uncertainty is introduced into the nuclear data used in the calculations due the temperature of the experiments. The temperature quoted in the experimental report for the core centre is 30±2C which gives a 10C difference between the calculation temperature and the experimental situation. Calculations were reported in Section 5.4 based on handbook data to check the effect

of a much larger temperature difference on k-effective for a similar type of system. It was found that the effect was very small (less than 0.02% change in k-effective). Based on this conclusion it is considered that the errors caused by the temperature difference between the calculation and the experiment for the present experiment can be ignored.

The first stage of the sensitivity analysis of the experiment consisted of performing additional MONK calculations in order to assess the sensitivity of the system multiplication to the following quoted uncertainties: critical height, critical width and length, Pu239 content, Pu240 content, U235 content, U238 content and H:(Pu+U) atom ratio. Note that the Pu239 and Pu240 content uncertainties are not independent as the residue of the total plutonium content is made up with the other nuclide in each case; a similar argument applies to the U235 and U238 uncertainties. Therefore, only the largest of the two values in each case has been included in the total uncertainty. Changes in the absolute level of plutonium and uranium are considered in the uncertainty in H:(Pu +U) atom ratio.

The sensitivity calculations were performed with a single case which was assumed to be representative of all the configurations. Consequently experiment 6.02 has been modified to provide the input for independent sensitivity calculations. Ten standard deviation increases were considered for all cases except 6.02C and 6.02F where, due to the relative size of uncertainty, increases of only five standard deviations were employed. The equivalent change in multiplication for a one standard deviation increase has been computed by assuming a linear relationship. The results of these calculations are given in Table 5.5.4 which shows that the total systematic uncertainty at the one standard deviation level is ± 0.0074 (0.74%) and is entirely dominated by the uncertainty in the Pu239 content.

The second stage of the sensitivity analysis consisted of assessing the uncertainties associated with the corrections made by experimentalists in deriving the clean critical dimensions given in the experimental report. These can be split into two components:

(i) The stacking voids and cladding

The experiments were performed by stacking the cladded fuel compacts to form three dimensional arrays. The corrections required to convert the experimental system into a clean configuration needed to take into account the cladding and the stacking voids. This was done by the experimentalists by evaluating the effect of multiple layers of cladding and void thickness and extrapolating back to zero in each case, based on linear relationship assumptions. A detailed sensitivity study on the effect of clad and stacking voids has already been made in Section 5.4 for a similar experiment performed at the same Laboratory, where it was found that the errors quoted in the experimental report were consistent with MONK calculations. It it therefore considered that the same conclusions apply for the present experiment and that an experimental uncertainty of the order of 0.0016 can be assigned due to stacking voids and cladding.

(ii) Conversion of Incomplete Layers of Compacts to Clean Dimensions

The other significant correction made by the experimentalists was the conversion of incomplete top layers of blocks and control rod insertion levels into corresponding clean dimensions. No assessment of the uncertainty in this correction is given in the experimental reports but it seems reasonable to assign a similar level of uncertainty as used for the stacking voids and cladding correction (0.0016).

Hence the total experimental uncertainty from the second stage of the sensitivity analysis is ±0.0023. Combining the uncertainties obtained from both stages of the sensitivity analysis gives a total experimental uncertainty at the one standard deviation level of ±0.0077 (0.77%)

(c) Comparison with MONK6B

Table 5.5.5 gives a comparison of the results for the seven experiments for the JEF2.2 library used with MONKDEV as reported above and for the current standard UKNDL-based library used with MONK6B.

As reported above the mean value for the JEF2.2 library calculations is 1.0323±0.0019. The mean value for the UKNDL calculations is 1.0250±0.0018. The differences between the two libraries is significant only at the two standard deviation level, with the UKNDL-based library apparently providing better agreement with the experimental measurements. In each case the UKNDL/MONK6B result is closer to the experimental result than the JEF2.2/MONKDEV result. The difference between both sets of calculations and experiment is significant at the three standard deviation level.

5.5.4 Summary

This report has shown that the Monte Carlo code MONKDEV over-predicts the average system multiplication for a series of critical experiments using Plexiglas-reflected PuO_2/ UO_2 / polystyrene blocks (8 wt% Pu240 in PuO_2, 0.151 wt% U235 in UO_2) with a 51.85 H:(Pu+U) atom ratio by 3.23%±0.19%. Correcting for the effect of temperature does not significantly effect the result for the seven cases. The calculated deviation from unity compares with an estimated total experimental uncertainty of ±0.77% (1σ). Thus the apparent positive bias on the mean calculated value is significant at the three standard deviation level. As the result for all of the cases is significant at the three standard deviation level, it is unlikely that the difference is due solely to a combination of experimental and calculational uncertainties.

The experimental uncertainty arising from the corrections applied to obtain the clean critical dimensions suggest that this set of experiments does not meet the full requirements of a benchmark experiment. However this set of experiments covers an important area of application that is otherwise poorly served by experimental data and so its inclusion is justified.

Table 5.5.1 - EXPERIMENTAL CRITICAL DIMENSIONS

Case No.	Number of Unclad Blocks		
	length (each block = 5.09cm)	width (each block = 5.08cm)	height (each block = 5.09cm)
6.01	8	8	7.156
6.02	8	9	6.462
6.03	10	10	5.188
6.04	10	12	4.787
6.05	12	11	4.562
6.06	12	12	4.429
6.07	12	13	4.340

Table 5.5.2 - SUMMARY OF MATERIAL DATA

Material	Density g/cm³	Nuclides Present	Fraction by weight %	Atomic concentration (10^{24} atoms/cm³)
Fuel - $Pu(8)O_2$ / $U(0.15)O_2$ / polystyrene	1.392	Am241 Pu239 Pu240 Pu241 Pu242 U235 U238 HinH2O O C	0.005 1.858 0.166 0.012 0.001 0.036 23.763 5.670 3.489 65.000	1.740E-7 6.521E-5 5.802E-6 4.177E-7 3.466E-8 1.285E-6 8.375E-4 4.719E-2 1.830E-3 4.540E-2
Reflector - Plexiglas	1.185	HinH2O C O	8.0 60.0 32.0	5.666E-2 3.570E-2 1.428E-2

Table 5.5.3 - RESULTS FROM STANDARD MONK CALCULATIONS

Case No.	k-effective - run1	k-effective - run2	Mean k-effective
6.01	1.0405 (0.0015)	1.0406 (0.0015)	1.0406 (0.0011)
6.02	1.0376 (0.0015)	1.0378 (0.0015)	1.0377 (0.0011)
6.03	1.0330 (0.0015)	1.0316 (0.0015)	1.0323 (0.0011)
6.04	1.0310 (0.0015)	1.0312 (0.0015)	1.0311 (0.0011)
6.05	1.0277 (0.0014)	1.0281 (0.0015)	1.0279 (0.0010)
6.06	1.0271 (0.0015)	1.0288 (0.0015)	1.0280 (0.0011)
6.07	1.0287 (0.0015)	1.0284 (0.0015)	1.0286 (0.0011)

The figure in brackets for the individual calculations is the standard deviation estimated by MONK. For the mean value the figure in brackets is the standard error on the mean value computed using the standard deviations from the two independent calculations.

Table 5.5.4 - RESULTS FROM MONK SENSITIVITY CALCULATIONS

Case No.	Uncertainty	Mean k-effective	Difference in k-effective from 1σ change
6.02	Reference case	1.0308 (0.0011)	
6.02A	Critical height	1.0371 (0.0011)	0.0006 (0.0002)
6.02B	Critical width and length	1.0341 (0.0011)	0.0003 (0.0002)
6.02C	Pu239	1.0671 (0.0011)	0.0073 (0.0002)
6.02D	Pu240	1.0148 (0.0011)	0.0016 (0.0002)
6.02E	U235	1.0308 (0.0011)	0.0000 (0.0002)
6.02F	U238	1.0289 (0.0011)	0.0002 (0.0002)
6.02G	H:(Pu+U) Ratio	1.0447 (0.0011)	0.0014 (0.0002)

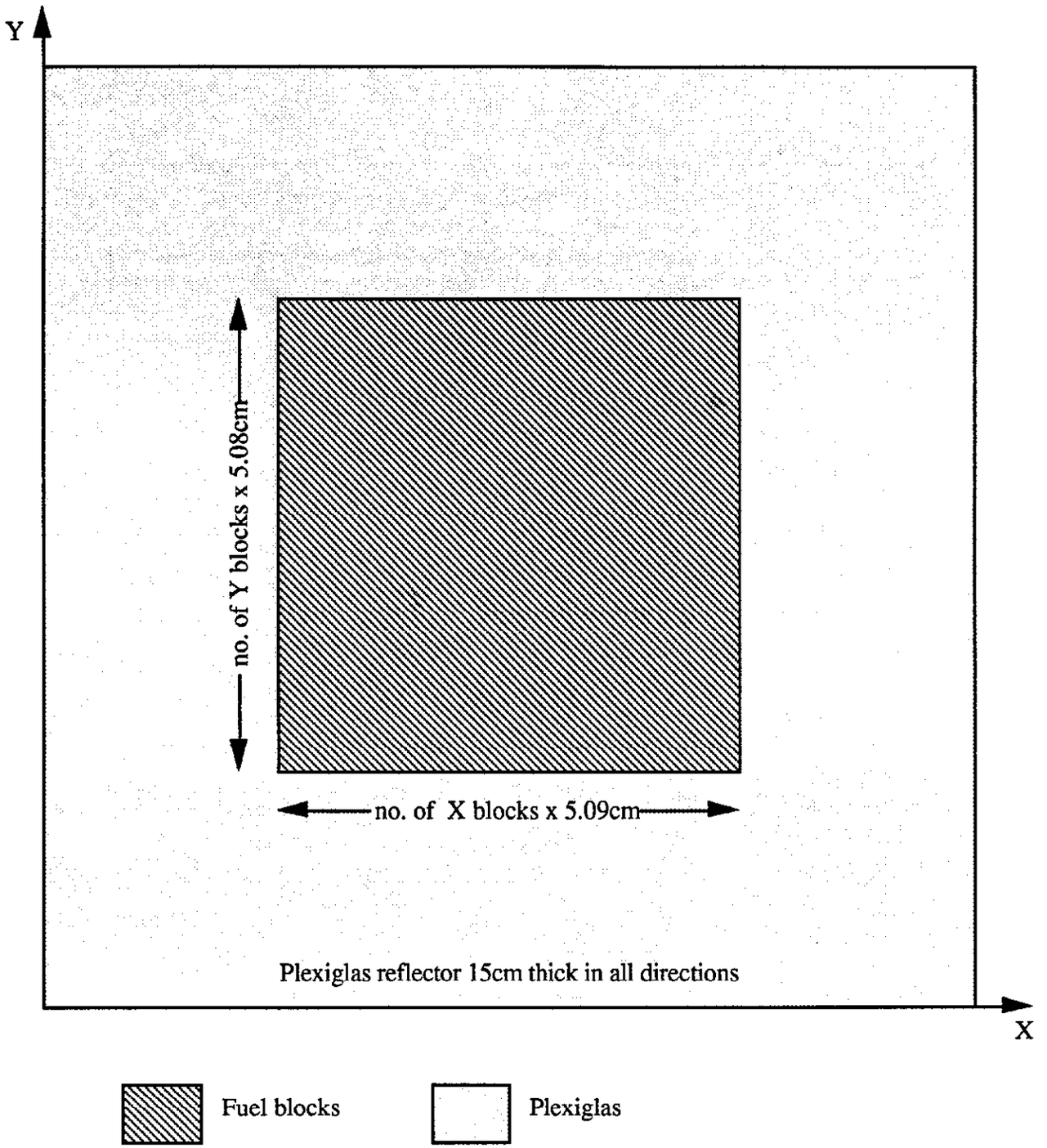
The figure in brackets in the mean k-effective column is the standard error on the mean value computed using the standard deviations from two independent calculations. The difference is computed by subtracting the reference case multiplication and scaling. The resulting standard error given in brackets.

Table 5.5.5 - COMPARISONS WITH MONK6B

Case No.	Mean k-effective - JEF2.2/MONKDEV	Mean k-effective - UKNDL/MONK6B
5.01	1.0406 (0.0011)	1.0319 (0.0010)
5.02	1.0378 (0.0011)	1.0308 (0.0011)
5.03	1.0323 (0.0011)	1.0249(0.0010)
5.04	1.0311 (0.0011)	1.0235 (0.0010)
5.05	1.0279 (0.0010)	1.0199 (0.0011)
5.06	1.0280 (0.0011)	1.0207 (0.0010)
5.07	1.0286 (0.0011)	1.0231 (0.0011)

The figure in brackets is the standard error estimated by MONK.

Figure 5.5.1 - PLAN VIEW OF THE MONK MODEL



Notes
1. Drawing not to scale
2. Dimension in Z direction = no. of Z blocks x 5.09 cm

6. CONCLUSIONS

This report has described the modelling of a selection of critical configurations from five experimental programmes using a JEF2.2-based nuclear data library in conjunction with a development version of the MONK Monte Carlo code (MONKDEV). Three of the experimental programmes concerned low-enriched UO_2 fuel in water, designed to support fuel storage and transportation applications. The remaining two programmes concerned plutonium systems, designed to support fuel processing operations.

For the well-thermalised low-enriched UO_2 experiments there is strong evidence to suggest that the JEF2.2-based library with MONKDEV can calculate k-effective within experimental uncertainties. This evidence is provided by over twenty configurations studied from three different experimental programmes performed at two independent laboratories. The slightly higher results obtained for the second experiment are probably as a result of the three different levels of moderation studied in that case, with the divergence from unity apparently increasing with spectrum hardness.

This suggests that the over-prediction for these under-moderated cases is due to epi-thermal data effects given the better agreement for the large quantity of well-thermalised cases from the three experiments. However it should be noted that the experimental uncertainty also increases with spectrum hardness for the second experiment and so one should be wary of drawing too firm a conclusion from the evidence available. Additional experimental studies for low-enriched UO_2 systems outside the well-thermalised range are planned in order to obtain further information.

In addition there is good evidence that the JEF2.2/MONKDEV combination produces more accurate results for the low-enriched UO_2 experiments than the current UKNDL/MONK6B combination. It is therefore concluded that for the types of low-enriched UO_2 systems studied here the JEF2.2-based library is acceptable from the point of view of calculating k-effective and is a useful improvement from the existing library.

For the two plutonium systems (although the fifth experiment considered mixed oxide compacts, Pu239 was the dominant fissile isotope) there was a marked difference between the performance of the JEF2.2-based data library. Experiment four was a very under-moderated system (H:Pu ~5) with an intermediate spectrum. The results for the configurations studied show a consistent over-prediction compared with the experimental uncertainties, in each case significant at the three standard deviation level. However the results also show a consistent improvement when compared with the UKNDL/MONK6B combination, where a significantly larger over-prediction was observed.

Experiment five was a much more well-thermalised system (H:(Pu+U)~50) and again demonstrated a consistent over-prediction compared with the experimental uncertainties, in each case significant at the three standard deviation level. However here the results are further from the experimental measurements than the UKNDL/MONK6B combination, due to a decrease in the thermal capture/fission ratio for Pu239. Such a decrease was observable in experiment four although due to the difference in spectrum the effect was smaller and compensated by other effects, most noticeably an increase in hydrogen capture at the upper end of the thermal range.

The results for the plutonium calculations suggest that although some improvements may have occurred in the intermediate range, the well-recognised problems with thermal Pu239 data are still causing significant differences between calculation and critical experiment measurements. Unfortunately the experiments studied here have relatively large uncertainties associated with them that serve to hide to some extent the calculational trends, but the differences between calculation and experiment are large.

Given the paucity of experimental data in this area the experiments used here, and others from similar programmes performed at the same Laboratory, will have a significant role to play in

validating new nuclear data libraries for criticality applications. On the basis of the evidence to date, there is no overall improvement in the calculation of plutonium systems to support the use of the JEF2.2-based nuclear data library from the point of view of calculating k-effective.

The analysis of additional experiments is planned with a range of hydrogen content, both employing plutonium in compacts as here or plutonium in nitrate solution, in order to obtain additional information of the use of the JEF2.2-based data for plutonium systems.

In summary the JEF2.2-based library when combined with MONK produces good agreement with critical experiment measurements for a range of low-enriched UO_2 systems that would be used to support its use in the criticality assessment of reactor fuel transportation and storage. Evidence exists of a tendency towards over-prediction for less well-thermalised systems but further data should be obtained. For plutonium systems the JEF2.2-based data when combined with MONK produces relatively poor agreement with critical experiment measurements, with significant over-prediction by the calculation in each case. Given the shortage of suitable critical experiments, and given the acceptability of an over-prediction from a criticality assessment point of view, it may prove difficult to improve matters in the short term. However further data should be obtained from modelling the limited number of other suitable plutonium systems in order to obtain a clearer view of the current status.

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