FUTURE DEVELOPMENTS IN CRITICALITY MODELLING AND DATA ANALYSIS IN BRITISH NUCLEAR GROUP

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Introduction

In 1989 in British Nuclear Fuels (as was) a variety of criticality assessment techniques were used, often starting with the use of a paper copy of a criticality handbook. Many survey calculations were performed using hand calculations or deterministic codes, such as WIMS [1]. The Monte Carlo code MONK [2] was used for more complicated models or to do cross-checks of limiting cases. A typical MONK run took around six hours with each input file yielding a single result.

In 2007 in British Nuclear Group Sellafield Limited (BNGSL) the starting point for an assessment is still often with the use of a well-thumbed paper copy of the same criticality handbooks. However, the criticality team now have a 100-core computer cluster that can run ten thousand Monte Carlo calculations in a six-hour period, all from a single input file.

Coupled with the increase in computer speed has been the development of code to support parameter sweeps, enabling a series of survey calculations to be performed from a single input file. MONK now contains options to vary a number of parameters within an input file. The stand-alone WORM code [3] presents similar functionality in a different format. CodeMore [4] was developed in BNGSL, as part of the NCD collaboration with Serco Assurance, to distribute parameter sweeps onto a computer cluster. This takes a single parameterised input file, converts it into the corresponding number of individual input files and efficiently distributes these across the computer network.

As part of an examination of potential improvements to the CodeMore system, the process of criticality modelling and analysis was reviewed to identify where changes had been made and whether full use was being made of current hardware and software capabilities. The overall aim was to identify further improvements that would free up the time of the criticality analyst to be better used for the most important step, i.e. analysis.

Input was sought from criticality analysts with experience ranging from the new graduate intake to those with thirty years experience. Involvement was also invited from members of the BNGSL code development team to provide an independent view of the process and advice on what could realistically be achieved. The review took account of developments being planned or under development in the UK code community as well as those relating to other criticality analysis packages.

Historically the criticality modelling and analysis process has involved a number of separate steps for the analyst, including:

1. *Translation of a design from engineering drawings into the corresponding criticality model in an input file.*
2. *Calculation of material specifications and transcription to the input file.*
3. *Checks of the input file using a visualisation package.*
4. *Submission of the input file.*
5. *Analysis of the output, including data manipulation and generation of graphs.*
6. *Iterative changes to the above process to determine 'optimum' values.*
7. *Peer review of each of the above steps.*

Although the introduction of parameterisation has removed some of the iteration from the process, it could readily be determined to contain areas for improvement. This paper outlines just a few of the ongoing and potential future developments along with some of the challenges that will need to be met before they are implemented.

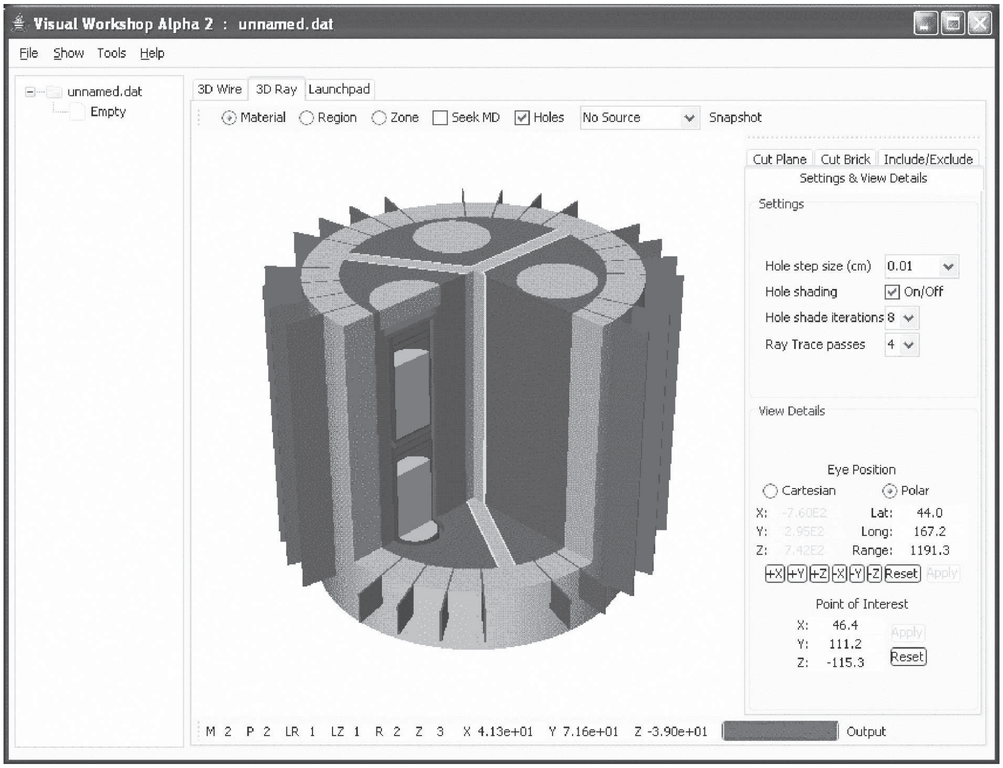
Creating Geometry Inputs and their Visualisation

Until recently the basic process for creating geometry inputs had changed little over most of the last two decades. Engineering drawings were passed to the criticality analyst, who converted the information from the drawing into a text based input file for the relevant computer code. The analyst used a separate visualisation package to view the geometry created and often only complete and error free inputs could be visualised. Therefore, the process of amending the input file and re-loading it into the visualisation package could be iterative and drawn-out.

There were some early developments in the visualisation field with the introduction of colour graphics packages – analysts in the 1980s would often check the model geometry using an alphanumeric representation.

In recent years simplified routes to define geometry inputs and provide visualisation have been under development. In the UK consolidation and further development of the functionality of three existing visualisation packages (VISAGE, VISTA-WIRE and VISTA-RAY) into a single new package, Visual Workshop, is taking place. This will enable the model geometry to be constructed and viewed using a single user-friendly graphical interface (Figure 1). Similar developments have been reported in support of KENO and MCNP [5,6]. The existing parameterisation formats are also planned to be superseded with an updated, more user-friendly format with enhanced functionality.

An obvious question to ask at this stage is why does the criticality analyst have to translate geometries between different formats? Drawings are now produced in Computer Aided Design (CAD) packages rather than on drawing boards. Links to CAD packages, to enable the criticality model geometry to be generated, manipulated *and visualised directly from the engineering drawing, have been investigated for several years. The model is then converted to a form that can be read by the criticality code. Several programs to convert from CAD models to MCNP already exist, and Serco Assurance has developed options to convert between CAD and MONK. An alternative route, tracking through CAD models, is currently being investigated for MCNP and MONK.*



Hole step size (cm) 0.01
Hole shading ☑ On/Off
Hole shade iterations 8
Ray Trace passes 4

○ Cartesian ● Polar
X: -7.60E2 Lat: 44.0
Y: 2.95E2 Long: 167.2
Z: 7.42E2 Range: 1191.3

Point of Interest
X: 46.4
Y: 111.2
Z: -115.3

```
M 2  P 2  LR 1  LZ 1  R 2  Z 3   X 4.13e+01  Y 7.16e+01  Z -3.90e+01   Output
```

Figure 1 - Example of Model Geometry within Visual Workshop

The use of CAD links may:

- *Allow direct criticality assessment of models generated using other assessment packages (e.g. finite element packages). This would enable more accurate assessment of complex models, e.g. deformation of fuel assemblies.*
- *Save user time in generating models and possible errors in translation, although this could require assessors to be able to use CAD packages to amend models.*
- *Enable the production of equivalent inputs for other codes, e.g. convert CAD input to MONK, MCNP, KENO or Attila. Such a tool may assist in promoting the use of these as cross-checks.*

There are still some issues to address with CAD links:

- *Conversion from CAD to MONK geometry is currently relatively slow although the resultant MONK model runs relatively quickly. If a conversion program was used assessors would not need to be able to use CAD packages.*
- *Currently tracking in CAD is much slower than in MONK. Hence, CAD would probably only be of benefit for fairly complex geometrical models where this could give additional detail over that available using MONK geometry options.*
- *Other teams have found problems with using CAD models in shielding assessments, particularly the issue of undefined volumes within the model.*

Existing and potentially enhanced tools enable the assessment of variations in an existing model. This can be split into three different technologies: parameter sweeps using CodeMore or similar programs; 'computational steering' i.e. user directed 'what-if?' modelling; and automated optimisation of the model to satisfy criticality criteria. The first of these, parameter sweeps, has become the de facto standard for criticality assessments within BNGSL. Optimisation, using genetic algorithms or hill climbing algorithms, has been investigated, using both MONK and the deterministic code WIMS, with promising results. Computational steering of criticality calculations is not used within BNGSL for a number of reasons, the primary one being the large amount of time taken by an individual Monte Carlo evaluation. Advances in computer technology will make computational steering a realistic possibility in the near future.

A possible long term development aim is an integrated modelling and assessment tool. From a basic CAD model either:

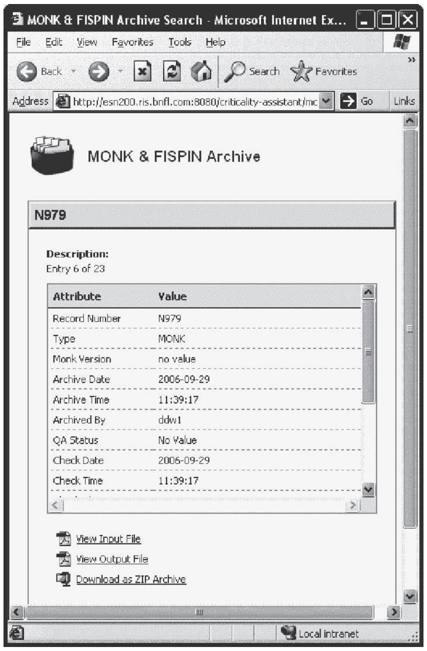
- *The k-eff shown on screen in real time as the designer changes the model (computational steering), or*
- *The model automatically refines itself to determine an optimum solution, or a range of parameter space that satisfies a set of pre-defined criteria.*

Such an integrated system may be a long way off although many of the components already exist.

A key requirement before these benefits can be *delivered is the availability of even higher performance computer systems. Traditionally these systems have been maintained in-house, however this limits the maximum number of CPU cores available. The availability of large external grids of computational resource may make this possible. The changes necessary to the CodeMore program to allow it to work with computational grids are currently being investigated.*

Data Storage - MONK Archiver

In the UK there is a requirement as part of the nuclear site licence that data relevant to the safety case of a facility is stored for the lifetime of a facility. With the introduction of parameterised input files and the generation of potentially thousands of relevant MONK calculations, compliance with this requirement produced a major challenge.



MONK & FISPIN Archive

N979

Description:
Entry 6 of 23

Attribute	Value
Record Number	N979
Type	MONK
Monk Version	no value
Archive Date	2006-09-29
Archive Time	11:39:17
Archived By	ddw1
QA Status	No Value
Check Date	2006-09-29
Check Time	11:39:17

View Input File
View Output File
Download as ZIP Archive

Figure 2 - Run details pane within the MONK Archiver

The MONK Archiver has been written to allow the criticality analyst to archive MONK inputs and outputs (runs). Runs are indexed using a combination of data extracted from the input and output files and optional user-entered data. This index is searchable and the analyst can quickly access runs selected on a number of criteria, for example containing particular key words and with certain limits placed on k-effective. Each run is given a unique number which can be referred to in a report. The use of web-technology enables this central archive to be accessed from the various BNGSL sites, with no data replication issues (Figure 2). The system is designed to be able to archive and retrieve surveys performed using parameterised files. Because it is necessary to be able to access the data in the future a neutral file format, based on eXtensible Markup Language (XML), has been used to store information about each run and for the index. The input and output files are stored in uncompressed 'zip' archives. Each zip file contains the input and output files, the index entry and an optional file from the MONKCheck program [7]. MONKCheck has been developed to extract key results from a series of output files and to identify any warning or error messages produced.

Common User Interface

One of the threads in the discussion above is the benefit of a common, user-friendly interface that links together all the individual software packages used to produce and visualise geometry, calculate material specifications and analyse and manipulate data generated in output files.

An ongoing development in BNGSL is termed 'Criticality Assistant', an umbrella term for a number of advances in the provision of timely information to the criticality analyst, delivered using internet technology. At its most basic the Criticality Assistant is a web site with a number of links to scanned documents and reports, for example ARH-600 and LA-12808. In this respect it differs little from other internet based resources such as CSIRC. What the Criticality Assistant also offers is web access to calculational routes and databases. In some cases new codes provide these calculational routes (e.g. the MONK Archiver), whilst in other cases the web interface calls pre-existing Quality Assured software. Re-use of existing software is extremely cost effective, and reduces the code base that needs to be maintained.

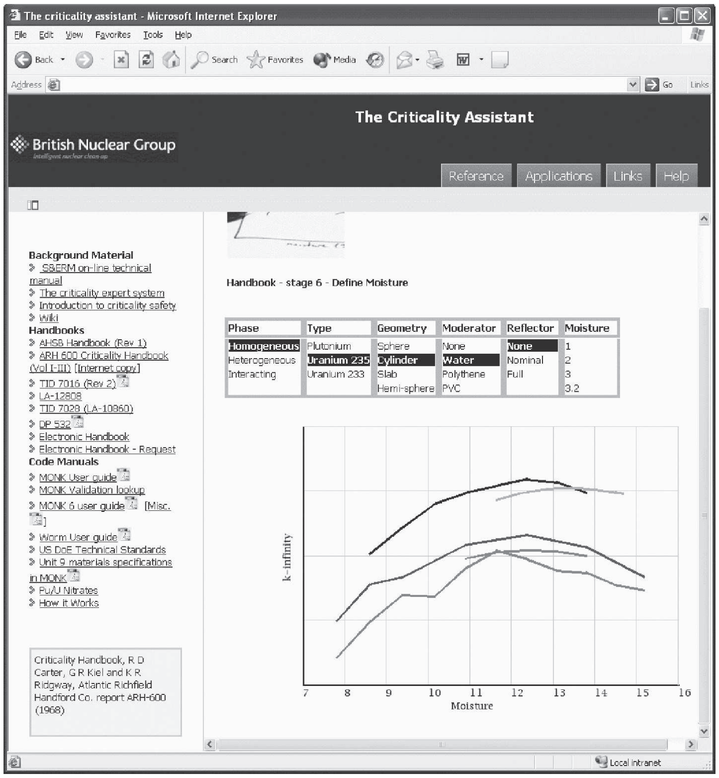
One of the options being evaluated is to provide an interface so that the user can specify the material variations they want in a simple, consistent format. Any interim calculations, such as conditions corresponding to 'fully saturated' would be evaluated by the code and this translated to the MONK input file. This approach, calculating the materials properties within the input file, means that parameter sweeps can be done using 'high level' quantities e.g. w/o water, with the individual nuclide weight percent being calculated automatically. This calculation can also consider geometrical changes to the system, e.g. PuO2 powder increasing in volume as further water is added to a fully saturated system.

A further development is in adopting the 'wiki' technology, of having a database of knowledge, freely editable by analysts. To this end the mediawiki software has been adopted as part of the Criticality Assistant. A quantity of existing information has been transferred to the wiki as a seed, and champions have been appointed to look after specific areas; however the content of the wiki is within the remit of the criticality and shielding staff within BNGSL. Care has been taken to differentiate the wiki information with the checked and quality assured data that underpins criticality safety methodology.

Application - Automated Generation of Handbook Data

A further application available on the Criticality Assistant is the provision of an electronic criticality handbook. Historic paper handbooks tend to contain data for specific bounding cases, e.g. fully water saturated material. While alternative data may have been generated for specific projects this may not be easy to locate. With an electronic handbook it is possible to investigate this data further, for example looking at bounding curves for keffective<1.

Data generated would be stored on a central database. The electronic handbook would enable a user to interactively search for relevant data and display this in various forms to gain a better understanding of the physical characteristics of a system (Figure 3). For example, data could be displayed as fissile mass vs. either moderator volume or fissile concentration for both critical and subcritical curves.



The Criticality Assistant

Background Material
- S&ERM on-line technical manual
- The criticality expert system
- Introduction to criticality safety
- Wiki

Handbooks
- AHSB Handbook (Rev 1)
- ARH 600 Criticality Handbook (Vol I-III) [Internet copy]
- TID 7016 (Rev 2)
- LA-12808
- TID 7028 (LA-10860)
- DP 532
- Electronic Handbook
- Electronic Handbook - Request

Code Manuals
- MONK User guide
- MONK Validation lookup
- MONK 6 user guide [Misc.]
- Worm User guide
- US DoE Technical Standards
- Unit 9 materials specifications in MONK
- Pu/U Nitrates
- How it Works

Criticality Handbook, R D Carter, G R Kiel and K R Ridgway, Atlantic Richfield Handford Co. report ARH-600 (1968)

Handbook - stage 6 - Define Moisture

Phase	Type	Geometry	Moderator	Reflector	Moisture
Homogeneous	Plutonium	Sphere	None	**None**	1
Heterogeneous	**Uranium 235**	**Cylinder**	**Water**	Nominal	2
Interacting	Uranium 233	Slab	Polythene	Full	3
		Hemi-sphere	PVC		3.2

Figure 3 - Electronic handbook data within the Criticality Assistant

Where data does not already exist the program would generate this automatically and add this to the database. To individually set up input files for each calculation, run these, extract results into a form where the data can be manipulated, present the data graphically and to check each step in the above would be very onerous. The aim is automate as much as practicable of the above process.

The project is ambitious in terms of its proposed functionality and flexibility. Various packages are being evaluated for the storage, manipulation and display of data, taking into account their ease of use and functionality.

Conclusions

Developments in computer hardware and software over recent years have provided significant benefits to criticality analysts. The benefits of these to a specific assessment are examined in more detail in a separate paper [8] and include:

1. *Faster and cheaper assessment process.*
2. *The ability to use a single parameterised input to analyse multiple variations of the basic model.*
3. *Better visualisation packages for computer models.*

The developments are intended to be tools to assist the criticality analyst, for example by freeing up time to spend on detailed analysis rather than simple data manipulation. It is important that the analyst truly understands the physics of a situation rather than relying on a series of results produced by computer codes. The behaviour of some systems may be difficult to predict and anomalies do occur. Training of analysts and the need for self review and peer review remains integral to criticality safety.

The review outlined in this paper indicates that while ongoing developments will provide further benefits to criticality analysts there remains much scope to further utilise future improvements in hardware and software. The items discussed above are still under development and feedback on these or experience of alternative approaches would be welcomed.

References

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2. *MONK: A Monte Carlo Program for Nuclear Criticality Safety and Reactor Physics Analyses, User Guide for Version 9, ANSWERS/MONK/REPORT/005*
3. *T Jones (2000), “WORM (Write Once, Run Many) A General Purpose Input Deck Specification Language”, Los Alamos report 99-3594*
4. *P Hulse and D Dewar (2006), “The Application of Recent Developments in Distributed Parametric Searches for Criticality Assessment Using the Code-More Program”, ANS 2006 Annual Meeting, Reno, Nevada, USA. 4th-8th June 2006*
5. *S M Bowman, B T Rearden, and J E. Horwedel (2005), “Complete User Visualisation Interface for KENO”, ANS 2005 NCSD Topical Meeting, Knoxville, Tennessee, 19th–22th September 2005.*
6. *R Schwartz (2006), “Visual Editor for Criticality Calculations Including Dynamic Source Convergence Assessment”, ANS 2005 NCSD Topical Meeting, Knoxville, Tennessee, 19th–22th September 2005.*
7. *K Searson (2003) “MONKCheck”, ANSWERS Seminar, 13th–15th May 2003. http://www.sercoassurance.com/answers/resource/areas/seminar/archive.htm [accessed 25th January 2007]*
8. *D Winstanley and M Nuttall (2007), “Criticality Design Considerations for a New Transport Package”, ICNC2007.*