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# MODELLING DROPPED RODS FOR CRITICALITY ANALYSIS

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## ABSTRACT

There are benefits in some criticality safety assessments of being able to analyse random arrays of rods in various vessels. This may provide a better indication of reactivity for a realistic situation compared to approximations (for example regular arrays of rods) that may be unduly conservative or indeed under-predict reactivity. This paper describes a method for generating a model and performing criticality calculations for such a random arrangement. The method has been implemented as a prototype development in the MONK Monte Carlo criticality code. The development uses existing facilities for particle tracking available in the MONK code, including the use of two different but complementary geometry packages, which employ different methods of particle tracking: simple body geometry and HOLE geometries. The use of both geometry models for this application has facilitated testing, particularly as the simple body geometry package includes in built self-testing routines. The algorithm for generating the array of rods first samples for a candidate rod, characterized by its location and orientation. The rod is then accepted or rejected depending on whether it satisfies the physical constraints of the system. In this manner, packing fractions of up to about 28% have been achieved with a rod length to radius ratio of around 10 to 1. The paper demonstrates that the algorithm is functioning correctly, and provides some comparisons with simplified modelling. The implementation makes use of the HOLE geometry option in MONK, which is widely used to facilitate the generation of complex geometries.

***KEYWORDS***: MONK, Criticality, Monte Carlo, Rods, Random Packing

## 1. INTRODUCTION

There are benefits in some criticality safety assessments of being able to analyse random arrays of rods in various vessels. This may provide a better indication of reactivity for a realistic situation compared to approximations (for example regular arrays of rods) that may be unduly conservative or indeed under-predict reactivity. If this arrangement is modelled using regular arrays of rods, then inaccurate criticality calculations may result. The purpose of the current work is to develop a method where the rods are modelled in a more realistic manner. To achieve this, a random arrangement of rods is first generated, and then particles can be tracked by using either simple body geometry models, or a new HOLE geometry (see below). The method described has been implemented as a prototype in the Monte Carlo criticality code MONK [1]. Over the last decade the development of MONK has been done as part of the Nuclear Codes Development (NCD) partnership between British Nuclear Group Sellafield Ltd and Serco Assurance, with the code being distributed and maintained by Serco Assurance's ANSWERS Software Service.

The ANSWERS software service provides a suite of codes used world wide for reactor physics, radiation shielding and nuclear criticality. Two of the major codes offered by ANSWERS, MCBEND and MONK are Monte Carlo codes that use a common geometry model for particle tracking. The MCBEND code [2] is used in the shielding area, whereas the MONK code is used for criticality and reactor physics.

The implementation of a random rod facility in MONK is related to other recent extensions for random placement of spheres that have been used for pebble bed reactor geometries [3]. A significant difference with rods compared to spheres is that orientation becomes an issue as well as location.

## 2. GEOMETRY MODELLING

The ANSWERS Monte Carlo codes use two different, but complementary, geometry models: simple body geometry and HOLE geometries. In simple body geometry, ZONES can be defined by the inclusion or exclusion of the simple bodies thus generating more complex shapes. Furthermore the bodies may be assembled into structures called PARTS. PARTS may be included within other PARTS and a given PART may be included in different positions within the geometry. In this manner models may be generated in a hierarchical fashion, allowing great flexibility in terms of detail and scale. To implement the simple body geometry, particles are tracked to boundaries where a change of material occurs. The code must calculate the distance to the ZONE boundaries in order to determine whether an event (such as a collision) takes place before the boundary.

A special type of PART is a structured PART. An example of such a structured PART is a CLUSTER PART, which consists of a containing body and a number of inner bodies that do not intersect with any other inner body, and are completely within the containing body.

The complementary geometry model is the use of HOLE geometries with Woodcock tracking. In this the mean free path used across the geometric region is the minimum from all the

materials, and the idea of fictitious as well as real events is introduced. After an event such as a collision occurs, the code determines what material the event has taken place in, and then decides if it is a real event or a fictitious event based on the ratio of the minimum mean free path to the real mean free path. In this manner, distances to boundaries need not be calculated, merely whether or not a point is within a body. This is often an easier task to perform. A number of HOLE geometries are built into the code, to represent in a flexible manner commonly occurring geometries. These include: the SQUARE HOLE which can be used to model a lattice of cladded rods, possibly surrounded by a square shaped wrapper; the GLOBE HOLE that can be used to model rods in a series of concentric rings, and so for example model an AGR fuel element; a PLATE hole which allows a number of materials to be modeled, separated by parallel planes.

Simple body geometry and HOLE geometries can be used together to good effect. In the paper we use both methods to model the random arrays of rods. Once the location and orientation of the rods has been generated, the simple body geometry can be used without further code modification. For the HOLE geometry, a new HOLE type has been implemented to model the random array or rods which we call the RANDROD HOLE.

## 3. MODELLING DROPPED RODS

To model the dropped rod geometry, the first stage is to generate the locations of the rods. It has been assumed that the layout can be simulated by rods with effectively random location and orientation. One way of achieving this is to successively add rods by generating a rod location and orientation, and accepting the rod if the rod lies within the containing vessel, and does not intersect with any previously accepted rod. Otherwise the rod is rejected. This process is continued until the desired packing fraction is achieved. This process has allowed packing fractions as observed in the target applications to be achieved.

The decision over whether two rods intersect is not completely straightforward, as a result of rod end effects. Whilst it is easy to determine whether infinite rods intersect, this is not the case for real rods and a number of special cases need to be examined in order to resolve the problem. (Even now in the implementation there are some cases where a rod is rejected when it could have been accepted.)

The question of whether a rod lies inside the containing vessel is less challenging, but still requires some care. In both cases, a numerical scheme is invoked to do the determination.

Once the rod locations and orientations have been determined, then a MONK calculation could use the existing features of simple body geometry referred to above to perform a criticality calculation. This requires no code modification. However, it may be more efficient to use a HOLE geometry. A HOLE geometry has been implemented as a prototype called the RANDROD HOLE, and the ability to model the configuration both in terms of simple bodies and HOLE geometries has facilitated testing. This is true both in terms of comparing final results, and testing whether the constraints on intersecting bodies etc. referred to above are satisfied. This latter facility is available because for a CLUSTER PART built in consistency self-checking can be invoked. This self-checking is based on a semi-analytic formulation of whether two simple bodies either intersect, or if one is completely contained within another.

In both the simple body geometry and the implementation as a HOLE geometry, the rods can be divided up further into radial zones for different materials. (In the case of the simple body geometry, the further refinement could be much more general by making use of the hierarchical nature of PARTs.) This allows, for example, a rod casing to be modelled.

### 3.1. Selecting a Rod

The first step in the sampling process is to select a candidate rod for inclusion in the model. The arrangement is shown in Fig 1.

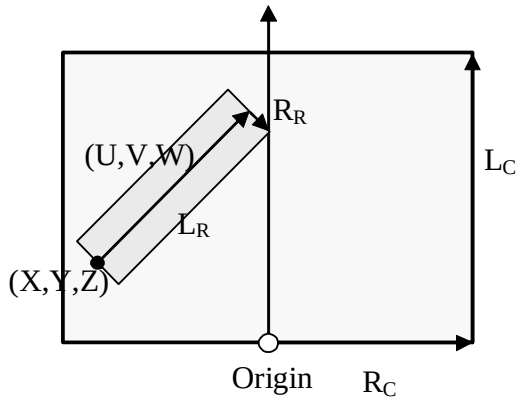


**Figure 1. Geometry of Rods and Vessel.**

Each rod is characterized by its length and radius, $L_R$ & $R_R$ (the same for all rods), the lower end of its axis (X,Y,Z) and the direction cosines of the axis (U,V,W). We therefore have to sample for U, V, W, X, Y, Z. This can be done by first selecting the orientation (U,V,W): randomly sample for the direction cosine in the vertical direction, W, from a uniform distribution in the range (0,1), then sample for the cosine and sine of the angle in the horizontal plane, C and S. We then can set U=C.Q and V=S.Q, where $Q=(1-W^2)^{1/2}$.

Once the direction cosine in the vertical direction is known, the axial range for the lower end of the rod is known, and so the Z co-ordinate can again be chosen from a uniform distribution, this time in the range ($R_RQ$, $L_C$-$L_R$W-$R_R$Q), where $L_C$ is the height of the vessel . The X and Y locations are both randomly sampled in the range ($-R_C$,$R_C$) where $R_C$ is the radius of the vessel. This choice for X and Y will include some rods that lie outside (either totally or in part) the containing vessel. The candidate rod is accepted or rejected based on the tests below.

### 3.2. Determining whether Rod lies Within the Container

The question of whether a rod lies within a cylindrical container can be determined by consideration of the origin of the rod and the direction cosines of its axis. The axial constraint is

automatically satisfied by the sampling method used for Z, so we only need to consider the radial constraint.

The radial constraint (that is $x^2 + y^2 < R_C{}^2$ for all points $(x, y, z)$ lying within the rod) can be checked by considering the two ends of the rod – if these discs both lie within the constraining cylinder then the whole of the rod does. In this case it is sufficient to look at the projection of the rod ends onto a plane perpendicular to the containing cylinder axis. This results in considering two ellipses with minor principal axes in the direction of the (projection of) the rod axis, and the major principal axes perpendicular to this rod axis. The problem than reduces to the 2D problem of checking that the two ellipses lie completely within a circle of radius $R_C$. We need only consider a quarter of each ellipse if we consider the region bounded by the two principal axes that point out of the container – formally the vectors defining these two directions satisfy the condition $\underline{x} \cdot \underline{u} > 0$, where $\underline{x}$ is the position vector of the centre of the ellipse, and $\underline{u}$ is the semi-principal axis. Considering only this quarter of the ellipse has the advantage that the maximum distance from the centre of the cylinder will correspond to the zero of the derivative of the distance with respect to distance around the ellipse circumference.

A numerical scheme can then be used to find the maximum distance of the ellipse from the origin, and hence whether the rod lies completely within the containing cylinder or not.

### 3.3. Determining whether Two Rods Intersect

The problem of whether 2 rods intersect is more complicated. If the rods were infinite in extent, then the problem would be straightforward. The minimum distance between the rods is along the common perpendicular of the rod axes. So if this distance is greater than twice the rod radius then the rods definitely do not intersect. On the other hand, if this distance is less than twice the rod radius AND the common perpendicular joins both rod axes within the physical extents of the rods, then the rods definitely intersect.

We are then left with some special cases to consider with regards the rod ends. We consider the four rod end faces (two from each rod) in turn, and consider whether the rod face intersects with any part of the other rod. If they do not, then together with the tests above, we can conclude that the rods do not intersect at all.

The intersection of the end of a rod with another rod of infinite length comes down to testing in 2D whether a circle intersects with an ellipse (by looking in a plane containing the rod end). We choose to reject the rod if any of the four ends would intersect with the other rod extended to infinity. This means that on occasion we will be rejecting a rod that could have been accepted (in the case of two rods being almost perpendicular, it may be that we are rejecting a rod based on another rod that is not even in close proximity). Nevertheless, for this application, we are not concerned about taking this modelling liberty.

### 3.4. Rod Placement Performance

Packing fractions up to about 28% have been achieved with this algorithm, when the rod length to radius ratio is of the order of 10 to 1. This value is adequate for the envisaged applications for the model. However it would be desirable to achieve higher packing fractions both for scoping calculation purposes, and also because the CPU time for rod placement increases dramatically as the limiting packing fraction achievable using the current algorithm is approached. Higher packing fractions are achievable, for example by including in the algorithm some subsequent movement of rods following placement. An example of this for Spherocylinders is described by Williams and Philipse [4].

## 4. TRACKING AND HOLE GEOMETRIES

The above section describes the algorithm for rod placement. The other part of the implementation is particle tracking, this is the subject of the current section.

The particle tracking techniques used in the simple body geometry package have certain potential limitations:

- Only bodies defined by equations that can be efficiently solved can be employed;
- Attempting to model certain replicating and complex components in a realistic manner can result in tracking inefficiencies due to the large number of boundaries involved;
- The task of composing and checking input data for such a model is a formidable one;
- Smearing out spatial detail introduces systematic errors of unknown size.

An alternative tracking strategy exists in the geometry package in the form of special HOLE materials, employing Woodcock tracking techniques. HOLE materials have been an essential part of the MONK code for many years and enable geometries commonly used in criticality analysis to be accurately and efficiently modeled. HOLE materials are used in conjunction with simple body geometries by placing a HOLE material inside a ZONE.

Tracking across body boundaries is necessary only because the mean free path varies between materials. If the mean free path could be made constant within a zone, then the tracking of boundaries could be replaced by the rather easier task of determining the material present at a collision point. This is the idea behind HOLE tracking, the mean free path is set equal to the minimum mean free path of all the materials in the HOLE, thus in general increasing the total cross-section. The device of increasing the total cross-sections introduces an additional artificial cross-section which in turn produces additional artificial collisions. The question of whether a collision is real or artificial is determined by sampling with a probability of a real collision equal to the actual material total cross-section divided by the total cross-section used for the tracking. The artificial cross-sections do not disturb the passage of the particle.

The spatial regions of the geometry of a HOLE material can themselves be filled with HOLE materials and these yet again to any desired depth.

The random rod geometry has been implemented as such a HOLE geometry (the RANDROD HOLE), which means it is possible to run calculations with the random array as either a

CLUSTER PART, or a HOLE geometry. One reason why HOLE geometries can give a big advantage over the solid body representation is because of the structured nature of the geometry. For example it is particularly easy, using properties of integer arithmetic, to describe the geometry of a regular array of rods with a HOLE geometry. This structure is not available to us in the case of a random distribution of rods, and to some extent, each rod must be tested individually to see if the collision site is within the rod. Therefore we cannot expect a speed improvement for the RANDROD HOLE commensurate with what would be achieved for a regular array.

Currently, following a collision, the code checks through the full list of rods to see if the collision has taken place within a rod. This is not an efficient way of solving the problem, and it is likely that dividing the region into sub-regions, each with its own sublist of candidate rods would improve the performance. However, results suggest that the rod placement algorithm dominates the code performance (certainly for high packing fractions with say several thousand rods to place), and it would be more effective to put effort into improving this part of the algorithm (see also subsection 3.4).

## 5. TESTING

The algorithm described above has been implemented as a prototype in the MONK code giving a new HOLE geometry (the RANDROD HOLE). By printing out the rod location and orientation in the correct syntax for MONK, the calculation can also be re-run using the simple body geometry package. This requires no further modifications to MONK, and so the particle tracking part of the RANDROD HOLE implementation can be tested against tracking facilities which have been established over many years, and are subject to rigorous testing. An example is given in the next section where the calculated $k_{effective}$ is given from equivalent calculations using a CLUSTER PART and the RANDROD HOLE, and it is seen that the calculations are in agreement.

A feature of the structured CLUSTER PART is that there are some in built geometry testing facilities. This geometry testing will check that none of the contained bodies intersect, and that all the contained bodies lie completely within the containing body. This is exactly what we require in order to check the rod placement algorithm. With only a few hundred rods, the self checking is quite quick. Nevertheless, a large 7000 rod case with a packing fraction of 28% was also checked with the CLUSTER part, and gave no failures. 28% seems to be about the limiting packing fraction that is achievable with this model.

The MONK code also has some associated graphics codes [5] which can be used to visualise the modelled geometry. The graphics codes read the MONK input, and generate the images using the actual tracking routines that are used for MONK calculations. This therefore also provides a good visual check that the geometry has been implemented correctly. One of the graphics codes, VISAGE, shows a slice through the geometry. Fig 2 gives an example case, showing a slice through a model, in this case with two vessels using the RANDROD HOLE. Two vessels were modeled in order to test and illustrate a number of additional features of the HOLE model, see below.

Each colour represents a different material. A small number of rods was modelled to aid visualization and to reduce the time to generate the image. In the real application, the packing fraction is much higher.

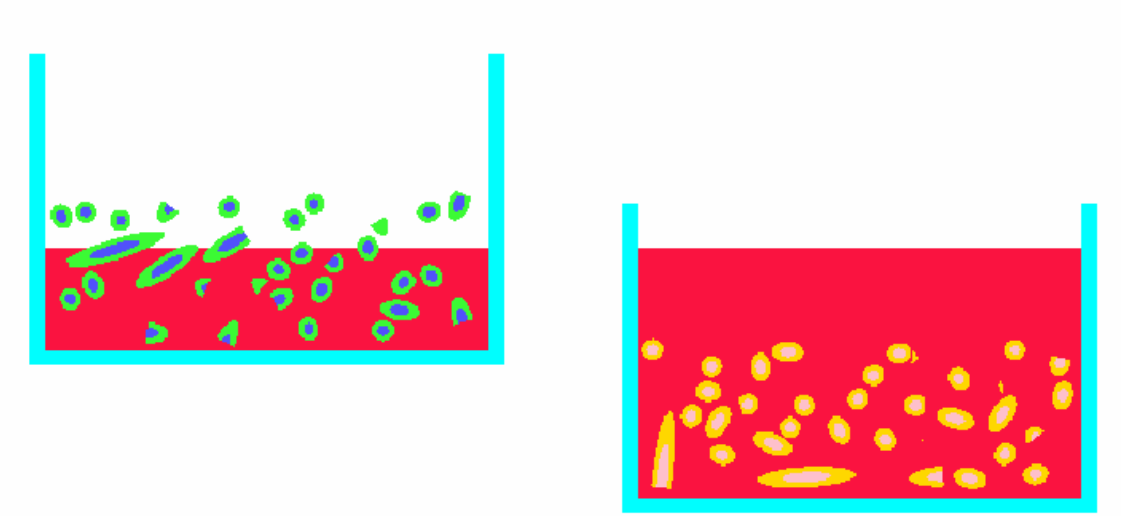

**Figure 2. Visualisation of RANDROD HOLE with the VISAGE graphics package.**

In the figure, the red material represents a fluid. Each rod is made up of 2 radial regions. The figure demonstrates that the modelling works correctly in that:

- changes of coordinates is working as intended,
- more than one HOLE geometry can be used in the same model,
- subsidiary HOLES work properly

This latter point is an important aspect of HOLE geometry. It allows the liquid level to be modelled as a PLATE HOLE, which is a HOLE where a number (in this case one) of parallel planes can be defined, with different materials between pairs of planes. It can be seen how this enables the fluid to surround the rods up to a specified level.

Another graphics package that is available from ANSWERS to visualize geometries is VISTA-RAY, which produces a three-dimensional image using ray tracing techniques. Fig. 3 shows an example.

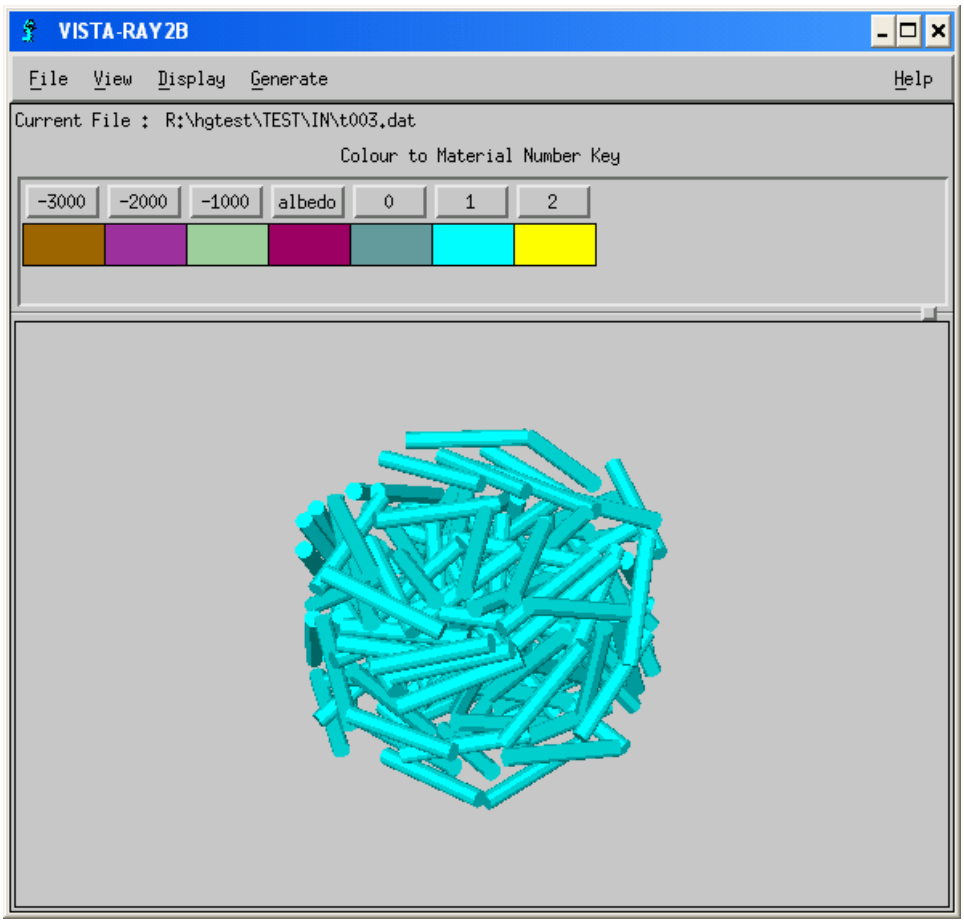


**Figure 3. Visualisation of RANDROD HOLE with the VISTA-RAY graphics package.**

## 6. RESULTS OF CALCULATIONS

This section gives some preliminary results from the random rod model described above. The purpose of the tests are:

- To confirm that the model is working correctly;
- To compare timings for the 2 geometry models;
- To give an indication of the effect of the new model.

The models in this Section used an artificial arrangement for testing purposes only. Two materials were used.

Material 1 Uranium, density 19 g/cc, 5% $U_{235}$ by weight, 95% $U_{238}$
Material 2 Water, density 1 g/cc

The first case presented consists of a cylinder with radius 150 cm and height 200 cm, filled with rods of length 100 cm and radius 7 cm. The rods were modelled as Material 1, and the interstitial material was Material 2. 150 rods were placed, corresponding to a packing fraction of 0.1634.

Before presenting the results, it is first helpful to show how $k_{effective}$ varies in this configuration, as the degree of mixing of the Uranium with water varies. This is presented in Fig. 4 below from a series of calculations where the Uranium is modeled as spheres on a regular tetrahedral lattice. The packing fraction is kept constant at 0.1634, but the diameter of the spheres are varied. (This uses one of the other HOLE geometries available in MONK, the T-HOLE.) In this instance, the spheres may intersect with the vessel boundary, in which case only the portions of the sphere within the boundary are used by the model.

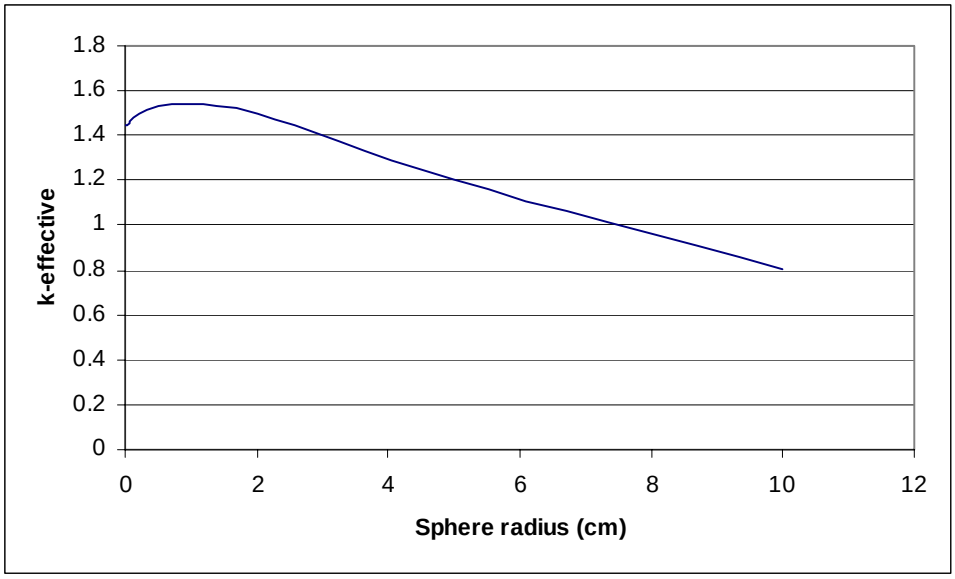


**Figure 4. Variation of $k_{effective}$ with mixing.**

Bearing in mind the shape of this curve, we now move on to the case with rods rather than spheres. In the case with rods, there are 3 differences in the modelling which may cause an effect.

- The Uranium is modeled as a rod, rather than a sphere
- All rods are completely within the vessel boundary
- The rods are arranged randomly both in terms of position and orientation, rather than as a regular array.

The results from the rod cases are shown in Table I below. Four calculations are given. The CLUSTER PART and the RANDROD HOLE should be equivalent in terms of the model. The GLOBE HOLE case models the rods as 75 rods of length 200 cm, arranged with vertical axes. This effectively models the 150 rods stacked as 2 sets of 75. The arrangement of these rods consisted of a central rod, then 4 rings of rods with 6, 12, 18 and 38 rods in each ring. The SMEARED Model uses the same total masses of materials as the other models, but modeled as a uniform mixture in the cylinder. It is equivalent to the case shown in Fig 4, as the radius approaches zero.

**Table I. Model Comparison, Test Case 1**

| MONK Model | $k_{effective}$ | σ | CPU (s) |
|---|---|---|---|
| **CLUSTER PART** | 0.8407 | 0.001 | 10266 |
| **RANDROD HOLE** | 0.8401 | 0.001 | 4949 |
| **GLOBE HOLE** | 0.7245 | 0.001 | 1600 |
| **SMEARED Model** | 1.4380 | 0.001 | 148 |

It can be seen that the results from the CLUSTER PART and RANDROD HOLE models are in agreement, but in this particular case the CLUSTER PART model takes just over twice the run time of the RANDROD HOLE model. It remains to be seen how this scales with number of rods modeled in industrial scale applications, and the result will also depend on the mean free paths in the various materials (relative to the geometrical length-scales).

There is a large difference in $k_{effective}$ between the rod models and a totally smeared case. This large difference is consistent with Fig 4 above. The equivalent sphere radius from the regular lattice case is about 9.5 cm, which seems consistent with the dimensions of the rods.

A further series of calculations were run using a packing fraction of 0.15. In this case the containing cylinder dimensions were: Radius 7.8528 cm, and height 80 cm. The rod radius was 0.5 cm, and the length used was (in three separate calculations) 20, 10 and 5 cm, corresponding to a number of rods 148, 296 and 592 respectively. These choices of dimension were used so as to allow for comparison purposes a 37 pin rod cluster (again using the GLOBE HOLE) 80 cm in length to be calculated using the same packing fraction. The results were as follows.

**Table II. Model Comparison, Test Case 2**

| MONK Model | $k_{effective}$ | σ | CPU (s) |
|---|---|---|---|
| **GLOBE HOLE** | 0.4939 | 0.001 | 205 |
| **RANDROD HOLE, 148 rods** | 0.4842 | 0.001 | 662 |
| **RANDROD HOLE, 296 rods** | 0.4873 | 0.001 | 887 |
| **RANDROD HOLE, 592 rods** | 0.4869 | 0.001 | 1445 |
| **SMEARED Model** | 0.4886 | 0.001 | 130 |

In this instance the parameter space for the calculations gave very little variation in $k_{effective}$ between cases. The comparison again confirms the general behaviour of the model, and also that the detailed modeling will not always be necessary.

## 7. CONCLUSIONS

A prototype model has been developed for the MONK criticality code to allow a random array of rods to be modeled for criticality assessments. The model allows the user to specify the number of rods, and for these rods to be positioned within a containing vessel to a desired packing fraction. The model generates the position and orientation of the rods in a way that does not allow the rods to intersect, and constrains all rods to lie within the vessel. Packing fractions up to about 28% have been achieved with the algorithm. The implementation of this model into an established criticality code means that the model can be used for industrial scale applications.

Two geometry models have been used, simple body geometry and HOLE geometry. The use of simple body geometry provides an independent check that the geometric constraints are satisfied by the rod position algorithm, and also that the evaluation of $k_{effective}$ in the HOLE geometry method is correct. The paper demonstrates the usefulness of HOLE geometries, and we note that in the course of the testing we have used three more HOLE geometries, the PLATE hole (for different materials separated by parallel planes), the T-HOLE (for an array of spheres on a tetrahedral lattice) and a GLOBE HOLE (for modelling a number of rings of parallel rods).

Idealised calculations have shown that the model is working correctly, and one example has been shown where the effect of the model is large, and another where the effect is almost negligible. It is anticipated that the model could be used in the nuclear industry to confirm or otherwise the adequacy of simpler models. If confirmation is not given, then the model can be used directly. However if the model is to be used for scoping calculations then improvements in speed are desirable, particularly for rod placement.

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## REFERENCES

1. N. R. Smith, M. J. Armishaw and A. J. Cooper, “Current Status and Future Direction of the MONK Software Package”, *Proc. Int. Conf. On Nuclear Criticality Safety, ICNC2003*, Tokai-mura, Japan, Oct. 20-24 (2003).
2. N. R. Smith et al, “The Current Status and Future Plans for the Monte Carlo Codes MONK and MCBEND”, *Proc Monte Carlo 2000*, Lisbon, Portugal (October 2000).
3. T. D. Newton, “The Development of Modern Design and Reference Core Neutronics Methods for PBMR”, *ENC 2002 Conference*, Lille, France, Oct 2002.
4. S. R. Williams, A. P. Philipse, “Random packings of spheres and spherocylinders simulated by mechanical contraction”, *Physical Review* E **67**, 051301 (2003).
5. M. J. Armishaw, A. Bird, H. Crofts, N. R. Smith, “The Role of Graphical Supporting Tools for Monte Carlo Analysis”, *Proc Monte Carlo 2000*, Lisbon, Portugal (October 2000).