

**METHODS AND CODES FOR NEUTRONIC CALCULATIONS
OF THE MARIA RESEARCH REACTOR**

K. Andrzejewski and T. Kulikowska
Institute of Atomic Energy, Poland

M.M. Bretscher, N.A. Hanan, and J.E. Matos
Argonne National Laboratory, USA

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ABSTRACT

The core of the MARIA high flux multipurpose research reactor is highly heterogeneous. It consists of beryllium blocks arranged in 6×8 matrix, tubular fuel assemblies, control rods and irradiation channels. The reflector is also heterogeneous and consists of graphite blocks clad with aluminum. Its structure is perturbed by the experimental beam tubes. This paper presents methods and codes used to calculate the MARIA reactor neutronics characteristics and experience gained thus far at IAE and ANL. At ANL the methods of MARIA calculations were developed in connection with the RERTR program. At IAE the package of programs was developed to help its operator in optimization of fuel utilization.

DESCRIPTION OF THE MARIA CORE

Geometry

One of characteristic features of the MARIA reactor core is its conical shape - see Fig. 1.

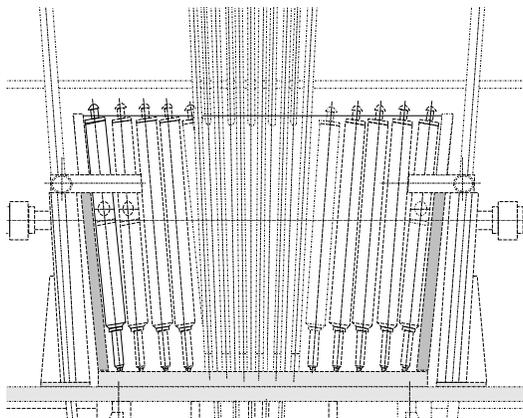


Figure 1 Vertical cross section of the MARIA reactor core

The transversal cross section of the core is given in Fig. 2, where its complicated structure can be observed.

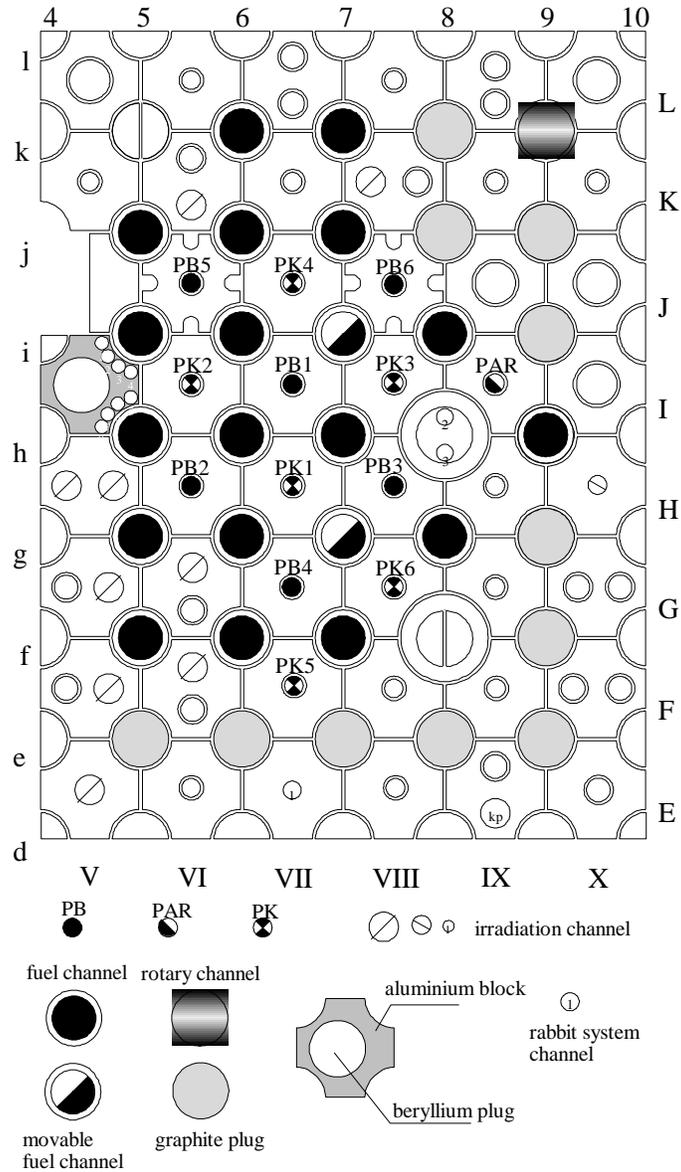


Figure 2. Horizontal cross section of the MARIA core

As can be seen, the beryllium matrix is assembled of 5 types of beryllium blocks with different effective water fraction. The fuel assembly channels may contain plugs of beryllium or graphite. The isotope production required further complication of the core with insertion of a special aluminium block. Taking into account that the fuel assembly is of tubular type - see Fig. 3, the neutron physics calculation with representation of the core details poses a serious problem.

At present the reactor is run on the remaining 80% fuel (see Table 1). The first critical experiment was performed in April 1998 with one 36% fuel assembly (with 550 g of U-235) loaded into the core, as a preparation for its future use.

The first operation period of the MARIA reactor lasted from 1974 to 1986. The period from 1974 to 1976 was a period of staff training and break-in of the new technical device. Between 1986 and 1994 the reactor was reconstructed to increase its safety. Operation was resumed in 1993. Operation times are given in Table 2. Since 1996 the reactor has been operated on a weekly cycle of 100 hours operation and 68 hours break. In each second or third cycle, the reactor has been shut down for economy reasons.

Table 2. Time table of MARIA operation in the years 1977 - 98.

Year	Number of hours	Year	Number of hours	Year	Number of hours
77	1413	83	3451	93	382
78	2294	84	3616	94	863
79	1967	85	2298	95	2180
80	723			96	2507
81	2215			97	3850
82	2437			98	est. 3120
Total	77-85	20414	Total	93-98	9052

METHODS AND CODES USED

Spectral Codes

For practical purposes the reactor was calculated using deterministic codes. The spectral calculations have been carried out using two versions of the WIMS code [2]: WIMSD-5 [3] at IAE and WIMS-ANL [4] at ANL. The following features of the codes have been utilized:

1. the Winfrith '86' library was used for WIMSD-5 at IAE and the ANL library based on ENDF/B-VI was used at ANL,
2. the Dancoff and Bell factors used in the resonance treatment for plate geometry were used in both cases using option 'TUBE' at IAE and 'supercell' at ANL,
3. the control rod cross sections were obtained by PIJ module at IAE, and as an auxiliary cell of the 'supercell' model at ANL,
4. the cross sections of nonfissionable materials were obtained by separate calculations in 'cluster' model at IAE, and as auxiliary cells of the 'supercell' model at ANL,

Global Calculations

For global core calculations the 3D transport code TRITAC [5] was used at IAE, the 3D diffusion burnup REBUS code [6] was used at ANL. Both codes are based on rectangular difference mesh.

Burnup calculations were performed in the macroscopic cross section option at IAE and in the microscopic option at ANL.

In both laboratories the deterministic approach was verified using the Monte Carlo MCNP-4 code [7], whenever necessary.

Transfer of cross sections from local to global codes

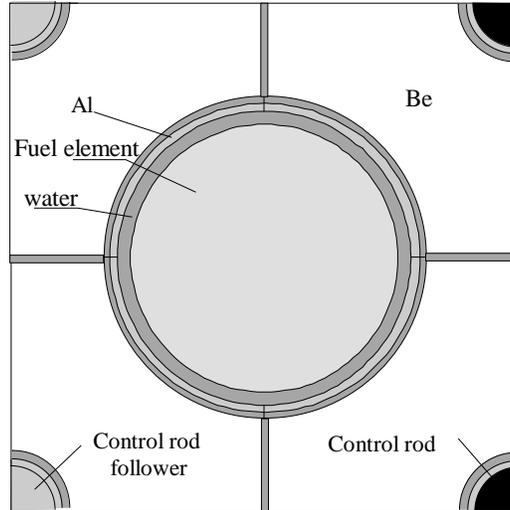


Figure 4. MARIA reactor elementary cell

In the global calculations, the fuel assembly together with the fuel channel tube and its water gaps are treated as a homogeneous medium. Beryllium blocks with their water gaps are treated as another separate medium. Control rods and their followers are also treated as separate media. All the media are eventually treated as rectangular zones in global codes.

The transfer of cross sections from spectral to global calculations at IAE required consideration of three effects:

- a/ error introduced by the WIMSD5 code when calculating cylindrical elementary cell
- b/ tubular structure of the fuel assembly
- c/ group condensation

In order to clarify the first effect, 4 model cells have been considered composed of a homogeneous fuel assembly region and beryllium moderator with geometries given in Fig. 5. A comparison carried out by MCNP has shown that the effect does not exceed 6 mk in k-inf.

The possible error caused as a consequence of the fuel tubular structure was treated by comparing two cases of reactor cell, both without control rods. First, k-inf of the elementary cell was calculated using WIMSD-5 and MCNP-4A codes with full representation of the 6 tubes in the fuel channel. Next, the calculations have been repeated with the contents of the fuel channel

represented as a homogeneous mixture of materials. In the first case the difference between WIMSD-5 and MCNP was 21 mk. In the second, the discrepancy was 3 mk.

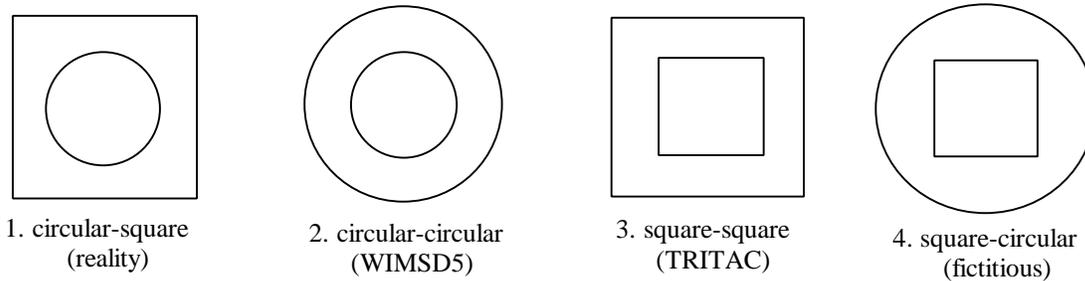


Fig.5. Possible schemes of fuel element and outer cell boundary

The difference between WIMSD-5 and equivalent TRITAC calculations is -12 mk, as a consequence of the condensation to 6-7 groups, homogenization of fuel assembly and change of the geometry. As a result, the systematic bias, relative to MCNP, of 33 mk in k-eff calculations of the core using the WIMSD-5 -TRITAC package is observed as a consequence of the condensation and homogenization of material constants for the tubular fuel.

Simplification of the vertical structure

The beryllium blocks used to form the reactor core matrix are of tapered shape, i.e. their largest cross section is 14×14 cm at the top of the core and 12×12 at the bottom. The evaluation of the influence of the slight slant of the blocks was treated with the MCNP code.

At IEA, two macrocells were compared using MCNP-4A. The first macrocell consisted of a single fuel assembly, surrounded by 4 quarters of the tapered beryllium blocks, with white boundary conditions at the macrocell boundary. In the second macrocell the beryllium blocks were assumed to have uniform dimensions in the vertical direction of 13x13 cm. The corresponding k-inf values for the macrocells were:

Elementary cell:	k-eff
Tapered blocks	1.63053 ± 0.00084
Rectangular blocks	1.63147 ± 0.00067

In the ANL calculation two full cores with 30 fuel assemblies were considered using the MCNP code. In the first core, the beryllium blocks were slanted and all 30 fuel assemblies placed taking into account their angle with the axes of co-ordinates. In the second, the beryllium blocks had parallel surfaces, and fuel assemblies were placed vertically. The corresponding k-eff values were:

Full core:	k-eff
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Tapered blocks	1.29229 ± 0.00016
Rectangular blocks	1.29233 ± 0.00013

The discrepancies between neutron fluxes calculated at three vertical positions in the core were as follows:

38 cm above core midplane	4.38%
at core midplane	0.42%
38 cm below core midplane	-6.41%

It was thus concluded, that the simplified model of the MARIA reactor, assuming parallelepiped shape of the beryllium blocks with the average cross section of 13x13 cm., may be used in further calculations

Influence of operational parameters on cell characteristics [8]

The influence of operational parameters on core characteristics was investigated using the spectral code, as these answers are needed to create the library of constants for global calculations. The results are as follows:

- a/ The variation of fuel temperature in the operational range results in 10^{-4} difference in k-eff and number densities during burnup.
- b/ The variation of the cooling water temperature in the operational range results in 10^{-5} difference in the above quantities
- c/ The variation of beryllium temperature from 50 to 90 °C results in 10^{-5} difference in U235 and U238 number densities during burnup and ~1% difference in k-eff.

It should be mentioned that for critical experiments, another set of data, calculated at 20 °C, was used. Calculation of burnup in 6 separate tubes and all the tubes treated as one material proved that up to 20% difference in U235 density can be observed between the innermost and outermost tube, but agreement on averaged quantities is very good.

Spatial models of the reactor

At IAE the 2D option of the TRITAC transport code was applied in global calculations to save computing time. The axial dimension was treated using buckling approximation. The effective bucklings were obtained from 3D calculations using the TRITAC code. A similar approach was used to represent the vertical position of the control rods. In transversal direction it was observed that the radial graphite reflector can be accounted for in a rather crude manner, without a significant loss of accuracy. The difference between full core k-eff calculations for 60 cm of graphite with 30 mesh points and for 30 cm of graphite with 5 mesh points is only 2 mk.

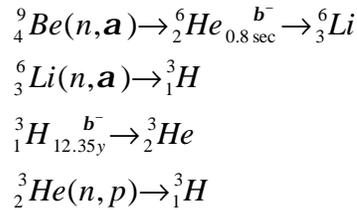
At IEA up to 15 different materials were used to represent different kinds of beryllium blocks with different poison water fractions. Three levels of He-3 and Li-6 poison were used to represent beryllium poisoning. At ANL two beryllium materials were used with averaged water fractions.

Two levels of He-3 and Li-6 poison were used, representing blocks with different irradiation history.

At ANL the 3D diffusion code REBUS was used for global calculations. The control rods were represented by internal boundary conditions at the rod boundaries. The dimensions of the control rods were suitably diminished in the square mesh to preserve the surface of the cylindrical control rods [9].

BERYLLIUM POISONING

The beryllium matrix of the MARIA reactor increases neutronic efficiency of the core due to (n,2n) reaction in beryllium. However, as a consequence of strong neutron capture of isotopes formed under irradiation in the beryllium, i.e. Li-6 ($\sigma_{th} = 720$ b) and He-3 ($\sigma_{th} = 4040$ b), the efficiency is reduced. The beryllium transformation chain looks as follows:



Li-6 is formed very quickly after absorption of a neutron in beryllium. The reaction cross section has a nonzero value only for energies above 0.74 MeV. Thus rate of production depends on the magnitude of the fast flux. Li-6 destruction is proportional to the thermal flux, and hence the saturation density of Li-6 depends on the fast to thermal flux ratio. Formation of He-3 is more complicated. Its concentration grows during reactor outages due to H-3 beta decay. Irradiation of He-3 during on-power periods reproduces H-3, to be decayed again during outages.

The effect of He-3 and Li-6 presence in the reactor cell is shown in Fig. 6 in the form of k-inf dependence on the number densities of the isotopes for the MARIA lattice with fresh fuel. The reaction rates of the above isotopes depend on the flux level and spectrum in the reactor which, in turn, depend on the following factors:

- the distance from the reactor core center,
- the distance from the fuel assembly within the beryllium block,
- the actual contents of Li-6 and He-3 in the block,
- the power level,
- the fuel burnup.

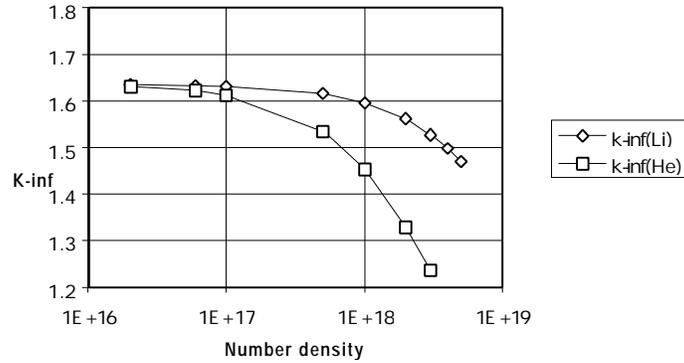


Figure 6. Effect of He-3 and Li-6 presence in the beryllium moderator on k-inf.

The influence of beryllium poisoning on MARIA cell characteristics was treated using an auxiliary program for solving the system of equations for number densities of isotopes involved in the transformation [10]. Reaction rates, which are coefficients of the equations, were obtained by WIMS, TRITAC and REBUS codes. As the effect is both spectrum and flux level dependent, the influence of all the above factors on beryllium poisoning had to be checked. It has been found that it is significant. For instance, at the end of 1986 the difference in He-3, Li-6 contents across the beryllium block is ~20%. At the beginning of 1995 the He-3 content in the blocks situated between fuel assemblies approaches $5E17$ atoms/cm³, while in those close to the graphite reflector were close to $9.5E15$ atoms/cm³. The respective numbers for Li-6 are $1.5E18$ and $5.6E17$ atoms/cm³.

The first period of the reactor operation has been followed by a several years' outage. During that period the amount of lithium remained constant but tritium formed during reactor operation decayed into He-3 with the decay constant equal to $1.78E-9$ sec. As a result, the average He-3 content for the blocks situated between fuel assemblies rose from $4.5E17$ to $3.4E18$ atoms/cm³.

The short breaks in reactor operation at the end of each reactor cycle are also important from the point of view of the poison formation. For instance, the He-3 content with detailed representation of core operating history is $9.2E17$ atoms/cm³ and with shutdowns neglected, the He-3 content was $6.7E17$ atoms/cm³.

On the basis of the above mentioned analyses, concerning both elementary cell and the whole beryllium matrix, it was concluded that further analyses of MARIA reactor should be performed using two beryllium zones in the matrix:

a/ inner - comprising beryllium blocks adjacent to the fuel

b/ outer - comprising blocks placed between the inner zone and the graphite reflector.

The exchange of poison number densities from values representative of the inner zone to the values representative of the outer zone, for a configuration of 1995, results in k-eff change of 7.5% $\delta k/k$ [10,11].

In the full core calculations, the number densities in the two, above determined zones, have been calculated taking into account detailed data concerning the reactor on-power and off-power periods. It was found recently, that as the poison formation is strongly dependent on the fluence of

neutron flux and the length of outages, it is also necessary to take into account periods of operation on lower than nominal power, usually not accounted for in yearly reports on the reactor operation. The latter approach with the two beryllium zones in the matrix has given the poison number densities, which introduced into the MCNP code gave $k\text{-eff} = 1.00150 \pm 0.00028$ for a critical experiment of February 1997 and 1.02421 using the REBUS code [9].

CALCULATION OF THE FIRST CRITICAL EXPERIMENT OF 1974

The first critical experiment of 1974 was used to test the actual accuracy of the methods and codes used at IAE and ANL as it is the only configuration of MARIA reactor not perturbed by beryllium poisoning.

MCNP-4 calculations

The calculations were performed for the geometrical model with full representation of fuel channels, beryllium blocks and graphite blocks. At IAE the MCNP capability of representation of repetitive structures was used. The vertical structure of the assembly is given in Fig. 7 below.

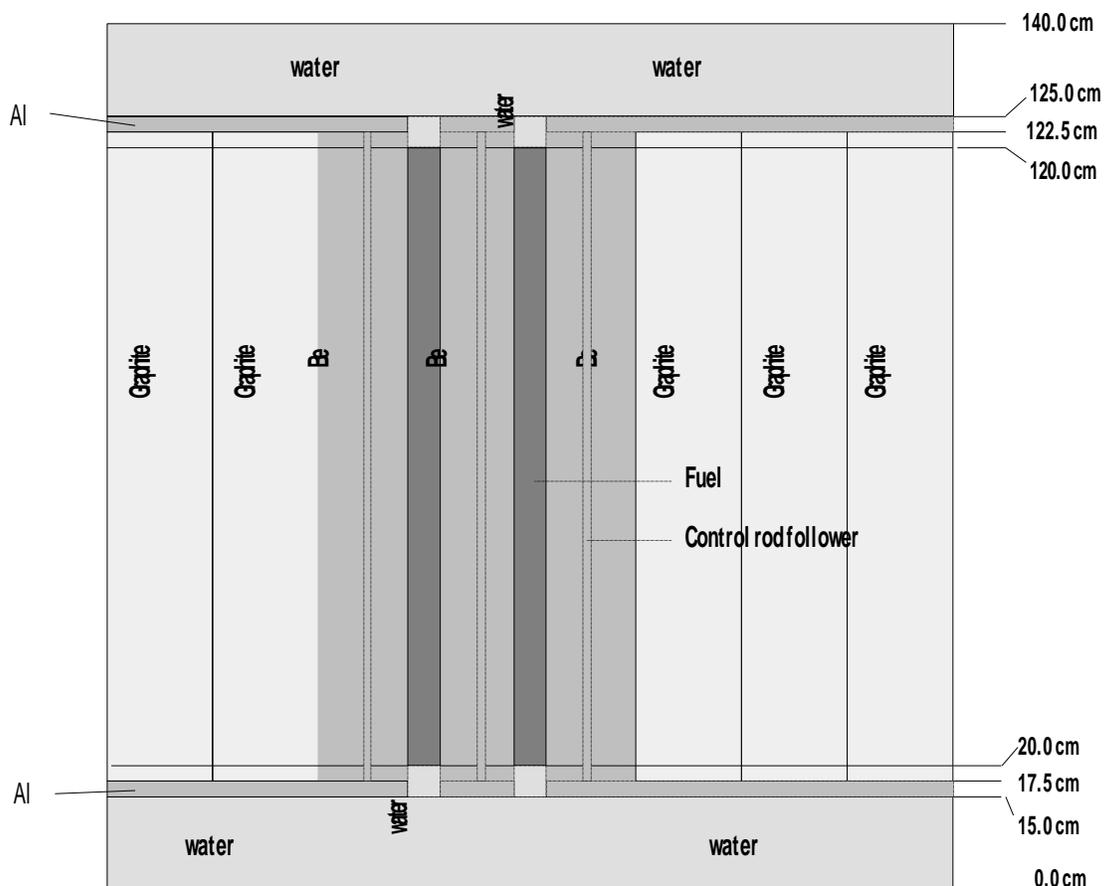


Figure 7. The simplified model of the fuel channel, beryllium block and graphite block in MCNP-4A

The IAE result is $k\text{-eff} = 1.01671 \pm 0.0028$. Further efforts to improve the axial model proved that the discrepancy in $k\text{-eff}$ is not caused by the axial model of the reactor. The computational model used at ANL differed from that used at IAE, i.e. the capability of repetitive structures was not used. The result is 1.0183 ± 0.0008 . As the two inputs are completely independent and the results agree within statistics, the discrepancy may be caused only by insufficient documentation of the experiment, e.g. description of water holes in beryllium blocks.

Deterministic calculations

The $k\text{-eff}$ obtained at ANL using the diffusion REBUS code for 1974 critical was 1.0426. This is consistent with the Monte Carlo results quoted above (~2% overestimate of criticality) and the diffusion theory bias [9], which is another ~2% in $k\text{-eff}$. Similar situation can be observed in 2D and 3D calculations using the TRITAC transport code at IAE. It is worth noting that the macroscopic absorption cross section of beryllium calculated by WIMS is negative for the highest neutron group to account for net neutron production as the consequence of (n,2n) reaction. This in turn distorts total cross section responsible for neutron transport. As a consequence the leakage from the system is underestimated, $k\text{-eff}$ and fast flux overestimated.

Conclusions

It has been proved that standard codes and methods are applicable to the highly heterogeneous MARIA reactor core. The accuracy of the standard methods and codes has been assessed. The accuracy of calculations of the main core characteristics has been established. Application of beryllium as the core matrix material requires special attention because of its poisoning by He-3 and Li-6, and unique neutron transport features.

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