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Mathematica as a Versatile Tool to Set-up and Analyze Neutronic Calculations for Research Reactors

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Abstract. Modern technical computing environments, such as *Mathematica* or *Matlab*, provide powerful tools and techniques for research reactor analysis combined with advanced graphical user interfaces. In addition, reactor calculations can now be efficiently supported by neutronics codes based on the Monte Carlo method due to the dramatic increase of computer performance in recent years. In particular for the analysis of very compact reactor cores, where an accurate three-dimensional model of the core becomes almost indispensable, Monte Carlo techniques are a very valuable asset.

In combining these approaches, we present a system that emphasizes an interactive interface based on *Mathematica*, while using standard burnup and Monte Carlo neutronics codes in the background (ORIGEN and MCNP). As an example, a generic single element reactor is discussed. The computational system is used to set up a complete MCNP model of the core, to optimize and prepare the input for burnup calculations, and finally to analyze the results of the calculations.

Attention should be drawn to the fact that the printed version of this publication is in black and white; all figures were, however, originally produced in color and can best be viewed with the electronic version of the article available at `web.mit.edu/aglaser/www/rertr2003/`.

Introduction

Reducing stockpiles of nuclear-weapons-usable materials present in the civilian nuclear fuel cycle and reducing the number of locations, where these materials are stored or used, are both of prime importance to strengthen global security. In this context, the conversion of research reactors from highly enriched to low-enriched uranium has recently received particular attention in the political and public debate. In particular, the U.S. committed itself to convert its remaining HEU-fueled reactors by 2012. Similarly, the new German research reactor FRM-II, the only HEU-fueled reactor built in more than a decade, is scheduled to use fuel of reduced enrichment by the end of 2010 at the latest. More generally, with the expected advent of advanced high-density fuels, every HEU-fueled reactor in the world should be able to use low-enriched fuel in the mid-term future. These developments offer a unique opportunity to end the use of HEU in the civilian nuclear fuel cycle entirely.

As a consequence, it is likely that activities to convert existing research reactors will intensify further and the need for corresponding neutronic calculations increase simultaneously. Especially, the analysis of the remaining high-flux reactors with a single element core may benefit from high-precision tools to adequately set-up and study reactor parameters using complete three-dimensional core models.

In this context, the use of modern technical computing environments can be very convenient for a variety of reasons: their analytical capabilities allow for a broad range of calculations and data manipulation, while their interactive graphical user interface facilitates intensive control of input parameters and interpretation of achieved results.

At the same time, Monte Carlo methods play an increasing role in neutron transport and burnup analyses. Even though, the use of such techniques is not necessarily recommended in every situation due to extensive requirements of computer time [Hanan et al, 2002], Monte Carlo methods offer the potential for high-precision modeling and analysis, in particular in the context of single element reactor conversion.

Below, a computational system is proposed that uses MCNP 4C [Briesmeister, 2000] for neutron transport and ORIGEN 2.2 [Croff, 1980/2002] for depletion calculations. Both codes are linked via MCODE, which has been recently developed at MIT. In the first part of the discussion, *Mathematica*[1] is used to set-up a complete research reactor core model,[2] while it is used in the final sections of this article to prepare and assist reactor burnup calculations.

[1] All calculations were performed with: *Mathematica*, Version 4.1.5.0 for Macintosh, System OS X. Wolfram Research, Inc. See also: S. Wolfram, *The Mathematica Book*, Fourth Edition, Cambridge University Press, 1999.

[2] An earlier version of this system was previously discussed in [Glaser, 2002].

Generation of an MCNP Input Deck

The fundamental idea of using *Mathematica* for reactor analysis purposes is to collect important operations in *Mathematica* functions and, hence, to focus the analyst's attention on the process of identifying the optimum model for subsequent calculations.

To this end, the user first collects the essential design information in a formatted list,[3] which can then be passed to the pre-defined functions made available in a package loaded at start-up of the notebook. In the case of single element reactors based on involute-shaped fuel plates, the following main functions are available to the user during the process of development and verification of the model:

- `PlotCore[coredata]`
- `GenerateInvolute[coredata, refpoints]`
- `PlotInvolute[points, coredata, paraboladata, circledata, zoom]`

The output of `PlotCore` and `PlotInvolute` is shown in Figure 1 for a set of sample design information. Additional data required for `PlotInvolute` are generated by `GenerateInvolute`, which approximates the involute defining the fuel plate by a combination of surfaces available in MCNP. The surface types used are paraboloids (SQ) for the inner part and cylinders (C/Z) for the outer part of the involute.

Once the user is satisfied with the accuracy of the surfaces proposed by the system to approximate the fuel plate, he or she can directly generate the corresponding MCNP input, which is written (to disk) by the following functions:

- `WriteMCNPCells[dirpath, mcnpinfo]`
- `WriteMCNPSurfaces[dirpath, surfacestrings, coredata]`

With the files of the cell and surface sections combined, a first executable MCNP file can be prepared by adding the cells and surfaces defining the surroundings of the core as well as the obligatory data cards defining materials, source, etc. At this stage, a first general analysis of the reactor can be performed with MCNP by adding the desired tallies to the input file. In particular, neutron spectra and flux levels can be determined conveniently with the present model.

A crucial property of any complex three-dimensional MCNP reactor core model is the accuracy of the total volume of those cells containing fissile material. In the present case, this value cannot be computed directly by MCNP due to the complexity of the used surfaces. To determine the fuel volume and, hence, the total fuel inventory in the core, the user can flood the voided model with neutrons from a homogeneous source

[3]The list (`coredata`) contains information on the inner and outer diameters of the core tubes, the thickness of meat and cladding, the width of the cooling channel, the fueled length, and the number and orientation of the fuel plates.

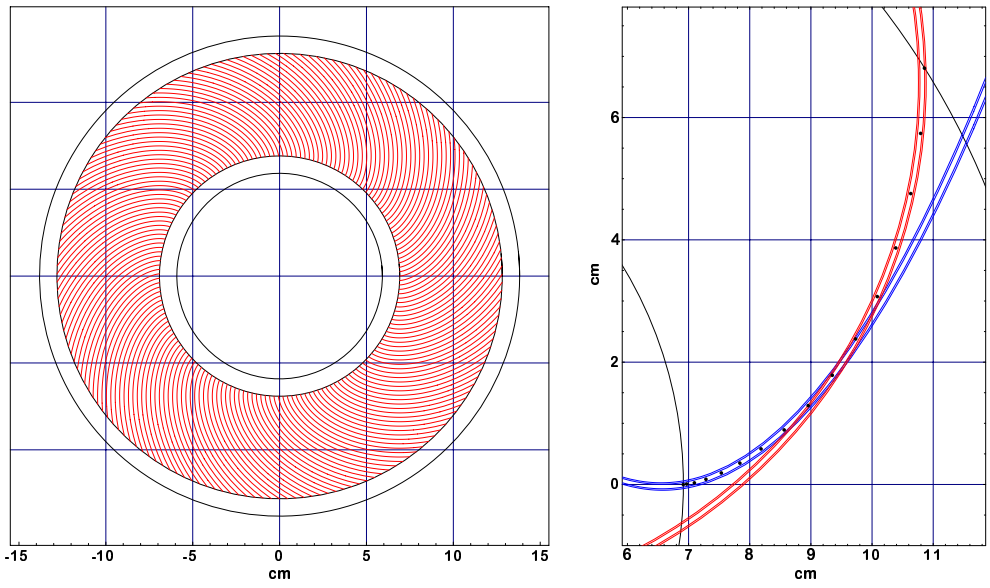

Figure 1: Results generated with *Mathematica* for an analysis of a single element reactor. Plot of fuel element generated with `PlotCore` function. Approximation of involute suggested by `GenerateInvolute` and plotted with `PlotInvolute`. Dots indicate the precise coordinates of the original involute. Shown dimensions are for the inner fuel element of HFIR.

and compare the value of a track-length (F4) tally in the cell of *unknown* volume with the value scored in a cell of *known* volume located nearby. If small deviations from the expected volume are revealed, the corresponding correction factor can be used to generate the final version of the core model in a second run of the *Mathematica* notebook.[4]

Preparation of Burnup Calculations

The fundamental advantage and main reason to use Monte Carlo methods for burnup calculations is the possibility to generate extremely accurate burnup-dependent one-group cross-sections and neutron fluxes for arbitrary core and fuel geometries. Yet, a set of values determined for a material at a given position and time remains accurate

[4]In general, the volume determined by the procedure described above is in excellent agreement with the expected value. In some cases, deviations in the order of 0.1% have been observed. The volume can be corrected by using a slightly "biased" value for the fueled length or the meat thickness during set-up of the model. The method for volume validation described above has been suggested by Nelson A. Hanan (ANL).

only in a local region, in which neutron spectrum and flux vary weakly — and only for a limited period of time, during which changes of the local isotopic composition are minor.

Since spatial effects are particularly pronounced for plate-type fuels used in compact reactor cores, a large number of burnup zones, i.e. of different material compositions, is indicated. However, while a fine burnup mesh is easily handled by deterministic codes, a very large number of zones of small volume, each containing a distinct material composition, becomes impractical for analysis with Monte Carlo methods.

The approach pursued here tries to combine the best of both worlds: it uses Monte Carlo techniques to determine burnup-dependent cross-section and flux data, while reducing the number of burnable materials to be treated explicitly in MCNP to a number manageable by the code. More specifically, the objective is to restrict the number of burnable material compositions to less than 100 — possibly even down to the order of 10 materials only.[5]

Generation of an Adaptive Cell Structure

Instead of having a regular — and strictly rectangular — structure with burnup zones of equal size, a characteristic adaptive cell structure is introduced here. The idea of such an adaptive cell structure is to join smaller areas within the plate with expected similar burnup behavior in one single burnup domain. The basic MCNP model generated with the procedure described above can then be updated and used for subsequent burnup calculations executed with a standard zero-dimensional burnup code.

As a template to select the characteristic cell structure, the power density profile in the fuel plate is used. This profile is determined with MCNP by subdividing the fueled region into very fine (typically several thousands) segments of equal volume. The corresponding additional input required for this procedure is again written by *Mathematica*, which also extracts the tally-data from the MCNP output-file once the simulation has terminated. Figure 2 (left) shows such a sample profile for a fuel plate having one discontinuity in the fuel density.

Once a template is available, an algorithm programmed in *Mathematica* is used to find a cell structure that approximates the given power density profile in the plate by rectangular segments, which can be handled by MCNP (Figure 2, right). The level of detail reproduced by the cells can be adjusted by a set of parameters and criteria of the search algorithm. Aside from the total number of desired MCNP cells, which

[5] In the following, for convenience, the term *material* is often used instead of *material composition* or *burnable material composition*. Note that each material typically consists of a large number of isotopes containing actinides, fission products, and fuel matrix.

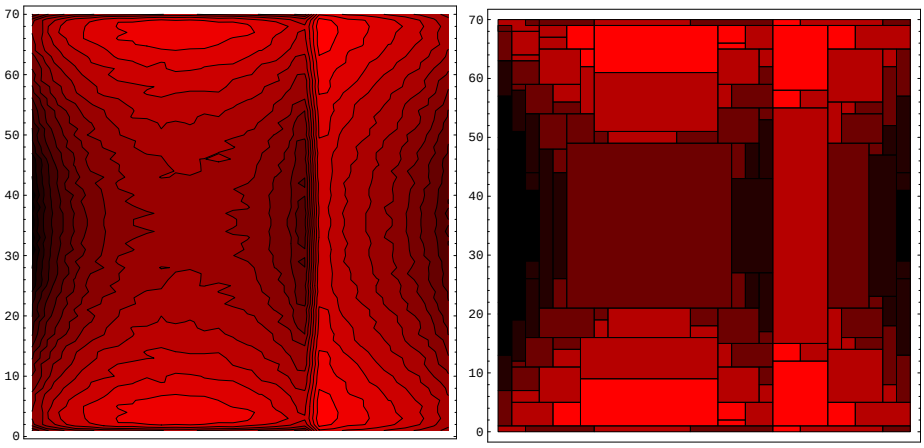

Figure 2: Power density profile (left) and optimized cell structure (right) for a generic fuel plate with one discontinuity in the fuel density. Dimensions of length and height of plate not to scale.

defines the "coarseness" of the structure and the sensitivity to variations in the local power density, the number of burnup zones and materials to be considered explicitly in MCNP are determined at this stage. Several cells are joined to form one domain, which will maintain the same material composition during subsequent burnup. Ultimately, *Mathematica* translates the cell data into MCNP syntax and writes the corresponding input to disk.

Burnup Calculations for a Generic Single Element Reactor

As an example for an application of the system to a practical analysis, a "generic single element reactor" is studied in some detail. The reactor model, which has been introduced and discussed elsewhere [Glaser and von Hippel, 2002], shows some typical characteristics of existing reactors in this category (see Table 1 for a comparison).

The core model is set-up with the *Mathematica* procedure described above, a power density profile generated in MCNP, and a cell structure for burnup calculations identified (Figure 3). In the present case, 9 domains — each containing one burnable material — are chosen for subsequent burnup calculations. As already indicated, each domain itself is constituted by a number of rectangular MCNP cells.

As outlined above, the ultimate objective pursued here is to perform burnup calculations with a standard zero-dimensional burnup code (ORIGEN), but with adequate sets of one-group cross-sections determined with MCNP specifically for the core being studied.

	RHF (ILL)	FRM-II	HFIR		Generic SER
Fuel type	UAl_x in Al	U_3Si_2 in Al	U_3O_8 in Al		UAl_x in Al
Enrichment	93 wt%	93 wt%	93 wt%		93 wt%
Thermal power	57 MW	20 MW	85 MW		30 MW
Uranium density [g(U)/cc]	1.17	1.5 and 3.0	0.78	1.15	1.50
Inner diameter	274 mm	130 mm	128 mm	286 mm	200 mm
Outer diameter	398 mm	229 mm	269 mm	435 mm	300 mm
Number of fuel plates	280	113	171	369	185
Active height of fuel plate	903 mm	700 mm	508 mm		700 mm
Thickness of fuel meat	0.51 mm	0.60 mm	max. 0.77 mm		0.60 mm
Thickness of cladding	0.38 mm	0.38 mm	0.25 mm		0.38 mm
Thickness of cooling channel	1.80 mm	2.20 mm	1.27 mm		2.00 mm
Total uranium inventory	9,200 g	8,108 g	9,430 g		6,627 g
Average power density in core	1,170 kW/cc	1,040 kW/cc	1,670 kW/cc		1,090 kW/cc
Coolant	D_2O	H_2O	H_2O		$\star$
Fuel element: center	$\star$	$\star$	H_2O Trap		$\star$
Fuel element: surrounding	D_2O	D_2O	Be-Reflector		$\star$

Table 1: Key characteristics of single element reactors.
Asterisks ($\star$) represent variable reflector, absorber, or coolant materials.

To perform this task, a computational link between the burnup code and the neutronics code has to be established. For this purpose, MCODE (MCNP-ORIGEN Depletion Program) has been used below. The program has been developed recently at MIT's Department of Nuclear Engineering and provides various improvements compared to other linkage codes available so far [Zhiwen Xu et al., 2002].[6]

To execute the burnup calculations, MCODE requires the initial MCNP input file of the core as well as a specific MCODE input file. The latter designates, in particular, the MCNP cells to be depleted, the number and position of depletion points, the ORIGEN libraries for those isotopes not explicitly treated by MCNP and provides information on the power density in the core and on the volumes of the cells.

$\star$

During each MCNP run, a new set of cross sections as well as new flux and power maps are determined. These data are then used for the next burnup step performed by ORIGEN. After completion of the last task, MCODE elegantly collects all relevant data produced in each phase of the simulation in a single output file. The output includes, in particular, reactivity vs. time and burnup, region averaged flux and conversion ratios, burnup and power maps, number densities as well as one-group cross sections

[6]The user's manual of the code has been included as Appendix B in: Zhiwen Xu: *Design Strategies for Optimizing High Burnup Fuel in Pressurized Water Reactors.* Ph.D. Thesis, Department of Nuclear Engineering, Massachusetts Institute of Technology, January 2003.

of actinides and fission products for each previously defined domain containing fissile material. MCODE also prints a sorted list of the neutron importance of all isotopes available in ORIGEN at EOL. The table can be used to verify that the most important nuclides are indeed considered explicitly in MCNP to account for neutron absorption — and not only in ORIGEN, which tracks the corresponding number densities for a much larger set of nuclides.

Some results for the generic single element reactor generated with the basic MCNP model as well as with the extended MCNP model, which was used in conjunction with MCODE to determine the expected cycle length of various core options, are illustrated in Table 2. Reactivity versus burnup is shown in Figure 4 for two fuel options of the generic single element reactor.

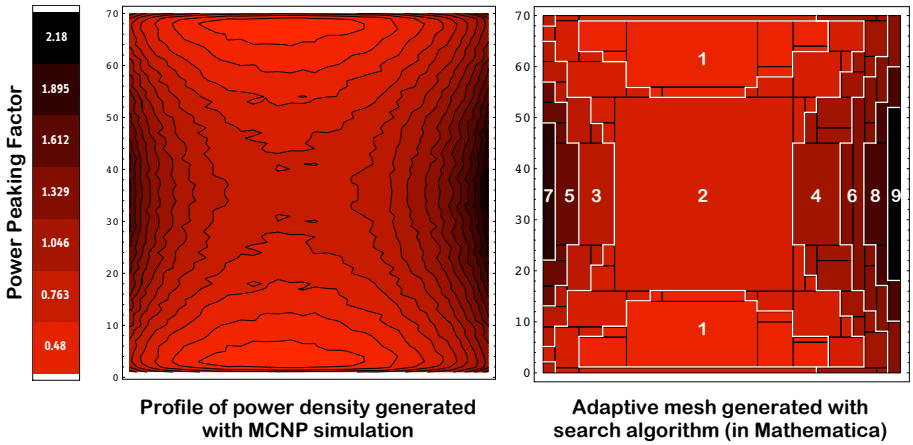

Figure 3: Adaptive cell structure for generic single element reactor. Domains 1–9 for subsequent burnup calculations are designated. Dimensions not to scale.

	HEU Design	LEU Core 1	LEU Core 2	LEU Core 3
Fuel type	UAlx Dispersion	UMo Dispersion	UMo Monolithic	UMo Monolithic
Enrichment	93 wt%	19.75 wt%	19.75 wt%	19.75 wt%
Thermal power	30 MW	30 MW	30 MW	30 MW
Uranium density	1.5 g/cc	8.0 g/cc	16.0 g/cc	16.0 g/cc
Inner diameter	200 mm	200 mm	200 mm	200 mm
Outer diameter	300 mm	300 mm	300 mm	300 mm
Active height of fuel plate	700 mm	700 mm	700 mm	700 mm
Thickness of fuel meat	0.60 mm	0.60 mm	0.60 mm	0.40 mm
Thickness of cladding	0.38 mm	0.38 mm	0.38 mm	0.48 mm
Thickness of cooling channel	2.00 mm	2.00 mm	2.00 mm	2.00 mm
Number of fuel plates	185	185	185	185
Fuel volume	4,418 cc	4,418 cc	4,418 cc	4,418 cc
Uranium-235 inventory	6,163 g	6,980 g	13,960 g	9,307 g
Coolant	Light water			
Fuel element: center	Beryllium reflector			
Fuel element: outside	Heavy water			
k(eff) at BOL	1.246	1.170	1.205	1.188
Max. th. neutron flux	9.82E14 n/cm2s (100%)	9.39E14 n/cm2s (95.6%)	8.46E14 n/cm2s (86.8%)	8.97E14 n/cm2s (91.3%)
Cycle length	60 days	37 days	95 days	56 days

Table 2: Sample results for "conversion" options of the generic single element reactor. LEU Core 3 is based on a reduced thickness of the fuel meat, compensated by an increased cladding. In all cases, it is assumed that EOL is reached when k(eff) = 1.05.

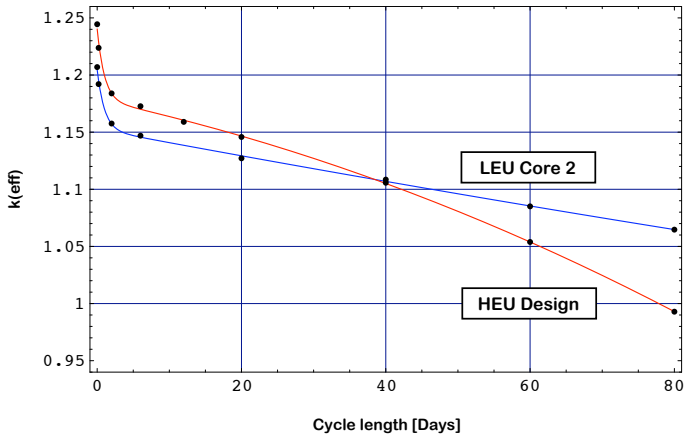

Figure 4: Reactivity vs. burnup for the original HEU design and LEU Core 2 of the generic single element reactor based on the 9-domain cell structure defined in Figure 3. Depletion calculations performed with MCODE. See Table 2 for details on the core and fuel options.

The level of detail of information obtained in the burnup calculations depend on the characteristics of the selected cell structure. Both the number of material compositions treated explicitly in MCNP and the number of MCNP cells used to describe the fuel plate determine the characteristics of the final results.[7]

For a given cell structure, the operational data and material properties in each domain of the fuel plate can be analyzed during burnup, in particular at EOL, and compared among each other as well as with the original data from BOL.

Domain	Power density at BOL	Power density EOL vs BOL	U-235 Burnup	Burnup discontinuity	Residual uranium enrichment
# 1	4.34 kW/cc	+17.2%	25.2 at%	9.3%	86.5 wt%
# 2	6.13 kW/cc	+9.2%	34.5 at%	8.2%	83.3 wt%
# 3	7.54 kW/cc	−1.7%	40.6 at%	6.1%	80.9 wt%
# 4	8.27 kW/cc	−4.0%	43.8 at%	8.2%	79.6 wt%
# 5	9.10 kW/cc	−11.8%	46.7 at%	5.8%	78.2 wt%
# 6	10.27 kW/cc	−17.2%	50.8 at%	6.6%	76.3 wt%
# 7	10.80 kW/cc	−22.6%	52.1 at%	5.4%	75.4 wt%
# 8	12.24 kW/cc	−27.7%	57.0 at%	5.7%	72.7 wt%
# 9	14.45 kW/cc	−38.5%	62.1 at%	5.1%	69.2 wt%
Average	6.79 kW/cc	±0.0%	36.6 at%	6.7%	82.2 wt%

Table 3: Variation of operational data in various domains of the fuel plate ordered from minimum to maximum burnup of fuel at EOL. Designation of domains according to Figure 3. Burnup discontinuity is the average delta to values in all adjacent domains at EOL. Averaged values for power density, U-235 burnup, and residual enrichment are weighted with the corresponding domain volumes.

Table 3 shows the variation of operational data in various domains of the fuel plate during burnup, i.e. the variation from BOL to EOL. The results obtained in the various domains, illustrate the high degree of local effects as expected for the given (very compact) core geometry. For instance, while the average uranium-235 burnup in the fuel plate at EOL is 36.6 at%, the maximum value exceeds 62% in a domain at the periphery of the plate, adjacent to the heavy water reflector surrounding the core.

In the current example, the average value of the burnup discontinuity, which describes the average burnup difference to adjacent domains, remains below 7% at EOL. If desired or required, this value could be reduced significantly, for instance, by subdividing domain #2 into one or more additional domains.

[7]Note that an increased number of (smaller) domains implies larger statistical errors of the MCNP tallies for a given computer time. Hence, the more burnable materials are treated explicitly in MCNP, the more computer time has to be assigned to maintain the same accuracy of the results because the average domain volume decreases correspondingly.

Outlook

Advanced technical computing environments provide powerful tools to facilitate the analysis and enhance the accuracy of neutronics calculations for research reactors. In the preceding discussion, we have developed a set of *Mathematica* routines to set-up and analyze calculations for research reactors of the single element type. MCNP is used for neutron transport and ORIGEN for burnup calculations, while both programs are coupled via MCODE to illustrate the efficiency of this concept.

An automated procedure to construct an extremely detailed three-dimensional model of the core with *Mathematica* as a basis for neutronics and burnup calculations was developed. Especially, the concept of an adaptive cell structure in the fuel plate, to be used for optimized burnup calculations, was introduced.

Further enhancements of the *Mathematica* routines are desirable and planned: in particular, the automated procedures to set-up MCNP input decks can be designed more comprehensively, facilitating the modeling of more general fuel types and core geometries. Improvements can also be made on the level of the construction of the cell structure for Monte Carlo burnup. In this case, an advanced procedure would allow a time-dependent evolution of the initially chosen cell structure. By adding this feature, the movement of control rods, and the corresponding impact on the burnup of the fuel, could be taken into account.

Also, an integration of the *Mathematica* routines required to prepare the cell structure for burnup calculations into pre-defined functions will be finalized. This would enable a user-friendly usage of the package — similar to the system already available for setting-up basic MCNP input decks.

Ultimately, the final computational system will be compared with other systems available for research reactor burnup calculations, for instance, based on diffusion codes — and by an application of the calculational system to existing reactors, where adequate operational data is available.

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