# ON THE ONGOING COMPUTATION OF THE LVR-15 REACTOR FUEL BURNUP

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ABSTRACT. Isotopic composition of the LVR-15 reactor fuel changes significantly during the operation time. In order to enable Monte Carlo calculations of the LVR-15 core throughout any reasonable time period, the isotopic compositions of partially depleted fuel assemblies have to be known at the start of the simulation. Even though the infinite lattice calculation can represent useful initial approximation, the non-leakage assumption is not necessarily valid for compact and highly heterogenous cores like in case of the LVR-15. Therefore, a more advanced calculation process have to be implemented towards appropriate determination of fuel assembly burnup. The main aim of this paper is to describe the current state of the ongoing computation as well as provide an explanation of the chosen calculation scheme of the LVR-15 operation history. Currently available results that are affected by profound inaccuracy are discussed in the final part alongside with planned future improvements.

KEYWORDS: Burnup calculation, Serpent, LVR-15 reactor.

## **1.** INTRODUCTION

The LVR-15 reactor [1] is a tank-type light water research reactor with 10 MW thermal power output. The reactor utilizes the IRT-4M 19.7 % enriched fuel and its main applications are material testing, silicon doping and production of radioisotopes.

Currently, the Serpent [2] computational model of the reactor is being developed with aim to perform its experimental qualification in the near future. One of the most crucial challenges concerning the development is a coverage of fuel burnup. There is an essential question of how to create proper representations of partially depleted fuel assemblies that are present at the start of an operation cycle.

In fact, there is a majority of fuel assemblies with nonzero burnup contained inside the LVR-15 reactor core at the beginning of each cycle. Therefore, determination of isotopic composition of partially depleted fuel have to be implemented in order to obtain convincing initial conditions that are needed for the Serpent calculation of any time step of any LVR-15 reactor cycle. The first obvious possibility is to calculate burnup-wise fuel isotopic concentrations in the infinite lattice approximation. However, it will be shown later that such approach does not have to be necessarily valid for compact and highly heterogenous cores with considerable neutron leakage. For this reason, a more advanced fuel burnup computation procedure has been applied.

The idea of this procedure is to take into account two important characteristics of the LVR-15 reactor. The first one is the above mentioned compactness and high heterogeneity of the core. The second one is the complicated operation scheme of the reactor, which involves short-term shutdowns in the run of a cycle operation. By adopting these two features, a more exact approximation in the fuel burnup implementation should be obtained.

This work is particularly focused on the introduction and description of the advanced LVR-15 reactor fuel burnup computation. The results presented in this paper are considered rather preliminary due to the fact that the computational process is still in the ongoing state. Nevertheless, the profound improvements will be realized on the basis of these first results in the following iteration of the fuel burnup calculation.

### **2.** Serpent model

The current version of the 3D Serpent model of the LVR-15 reactor allows to build the reactor model with any desired core configuration that contains the most frequently used components, i.e. fuel assemblies, beryllium blocks, water displacers and irradiation channels. All components in the core are surrounded with water and placed inside the reactor vessel. An instance of a core configuration geometry plot of the Serpent model is provided in Figure 1.

As for fuel components, both standard 8-tube and control 6-tube IRT-4M fuel assemblies can be chosen. Control rod positions are adjustable according to the demanded pattern. In addition, both fuel assemblies can be defined with a variety of possible burnup distribution structures. Different fuel material compositions can be assigned to corresponding regions of a particular fuel component using these distribution structures.



FIGURE 1. Serpent geometry plot of the opening LVR-15 core configuration of the K216 cycle; two fuel assemblies with initial zero burnup are highlighted (standard 85A710 – red, control 65C666 – black).

The initial fuel burnup implementation is based on burnup-wise isotopic compositions of standard fuel assembly calculated with Serpent in axially and radially infinite lattice. The Serpent model utilizes predefined burnup library with atomic densities of considered nuclides as functions of burnup (see Table 1).

#### **3.** Computational process

The chosen process of the burnup computation is based on the real operation scheme of the LVR-15 research reactor. The complexity of the reactor schedule is emphasized in Figure 2 and Figure 3, where powers and  $k_{\text{eff}}$  from Serpent are visualized, respectively.

More than a 2.5 year latest time period of the reactor operation has been considered for the purpose of the computation. This time interval was determined according to the moment when a fuel assembly with the largest burnup in the currently running cycle has been introduced into the reactor core for the first time as a fresh fuel component. This condition is fulfilled by the K216 cycle, where two new fuel assemblies have been added into the operation procedure – one standard (85A710) and one control (65C666). The position of the former is marked with red colour, while the latter is highlighted with black colour in terms of the K216 core layout visualization in Figure 1.

The whole computational process consists a total of 14 operation cycles starting from the K216 up to the K229. Two fresh fuel assemblies in average are introduced into the reactor core at the start of each of the examined cycles. Since that point, burnup development of these fuel assemblies can be calculated without the uncertainty in the fuel material composition. This presumption is supported by the fact that the fresh fuel assemblies have known initial isotopic concentrations. Overview of fuel assemblies with this attribute is listed in Table 2 alongside with the information whether any particular fuel assembly was present in the corresponding operation cycle.

The computational process of the latest operation history of the LVR-15 reactor has been designed on the basis of data from the nodal code that is used for cycle designing at the LVR-15 [3]. These data come from nodal calculation of given cycle that has been carried out with genuine operational power data of the reactor. A typical calculation schedule of the LVR-15 reactor cycle contains over a hundred partial critical calculation steps. That reflects the complexity of the reactor operation.

The same approach has been adopted in the Serpent based computational process in order to achieve authentic operational conditions of the LVR-15 reactor as closely as possible. As for initial step of the entire computation, referred as the step 0 of the K216 cycle, the material compositions of fuel assemblies with nonzero burnup have been obtained from the above mentioned infinite lattice burnup library implemented in the Serpent computational model. Axial-wise burnup data divided into 5 regions of these fuel assemblies have been taken from the calculation of the previous K215 cycle from the operational nodal code.

The scheme of the computational process is expressed in Figure 4. A single step of the computation other than the initial step 0 of the K216 cycle can be described with a sequence of the same partial procedures. First, the appropriate operational data of the LVR-15 are loaded and transformed into the *input* file that is needed for the building of the corresponding LVR-15 reactor Serpent model. These data include:

- the name of the current cycle,
- the calculation step number in the cycle,
- time interval length of the step,
- reactor power during the calculation step,
- identifiers of present fuel assemblies,
- core configuration layout within the step,
- control rod insertions in the step core layout,
- specifics of uranium targets in the core centre.

In addition to the *input* file, the second set of data has to be provided. The second set contains calculated isotopic compositions of fuel assemblies from the previous step. This data stream is referred as the *oldDepFile* and it is sent to the *slvr15* together with the *input* file. The *slvr15* procedure represents a software tool designed for creation of the Serpent input file of demanded configuration of the LVR-15 reactor

80160	130270	420950	430990	441010	451030	471090	481130	531350	541350	551330
551340	551350	601430	601450	611470	611490	611510	621470	621490	621500	621510
621520	631530	631550	641550	641570	922340	922350	922360	922380	932370	942380
942390	942400	942410	942420	952410	952430	962430	962440	962450		

TABLE 1. List of 42 considered nuclides that are passed on between subsequent computation steps (ZAI numbers [4]).

	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229
85A710	×	×	×	×	×	×	×	×	-	×	×	×	×	×
65C666	×	×	×	×	×	×	×	×	×	×	×	×	×	×
85A711	-	×	×	×	×	×	×	×	×	×	×	×	×	×
85A712	-	×	×	×	×	×	×	×	-	×	×	×	×	×
65C667	-	×	×	×	×	×	×	×	×	×	×	×	×	×
65C668	-	-	×	×	×	×	×	×	×	×	×	×	×	×
85A713	-	-	-	×	×	×	×	×	×	×	×	×	×	×
85A714	-	-	_	×	×	×	×	×	×	×	×	×	×	×
65C669	-	-	-	-	×	×	×	×	×	×	×	×	×	×
85A715	-	-	-	-	-	×	×	×	×	×	×	×	×	×
65C670	-	-	_	_	_	×	×	×	×	×	×	×	×	×
65C671	-	-	_	_	_	-	×	×	×	×	×	×	×	×
65C672	-	-	-	-	-	-	×	×	×	×	×	×	×	×
85A716	-	-	-	-	-	-	-	×	×	×	×	×	×	×
65C673	-	-	_	_	_	-	_	×	×	×	×	×	×	×
85A717	-	-	-	-	-	-	-	-	×	×	×	×	×	×
85A718	-	-	_	_	_	-	_	_	×	×	×	×	×	×
65C674	-	-	_	_	_	-	_	_	×	×	×	×	×	×
65C675	-	-	-	-	-	-	-	-	-	×	×	×	×	×
85A719	-	-	-	-	-	-	-	-	-	-	×	×	×	×
85A720	-	-	-	-	-	-	-	-	-	_	×	×	×	×
85A721	-	-	-	-	-	-	-	-	-	-	-	×	×	×
65C676	-	-	-	-	-	-	-	-	-	-	-	×	×	×
60C834	-	-	-	-	-	-	-	-	-	-	-	-	×	×
60C835	_	—	_	_	_	—	_	_	_	_	_	_	×	×
85A722	_	—	_	_	_	—	_	_	_	_	_	_	_	×
85A723	-	-	-	-	-	-	-	-	-	-	-	-	-	×

TABLE 2. The presence of initially fresh fuel assemblies throughout considered cycles K216–K229 (× in the cycle, – not in the cycle).



FIGURE 2. Power sequence of the LVR-15 reactor operation including cycles K216–K229.



FIGURE 3. Development of  $k_{\rm eff}$  calculated with Serpent throughout cycles K216–K229.



FIGURE 4. Scheme of the computational process.

computational model. The main input file is prepared for the Serpent calculation of particular step of the computational process after the slvr15 execution. One of the step calculation outputs is the Serpent depletion file indicated as the NewDepFile. This output file alongside with appropriate operational data is used as the input for the calculation of the following step. The introduced process is repeated n times according to the number of steps in the whole computation.

The isotopic composition of fuel assemblies between subsequent steps is passed on for 42 selected nuclides. The list of considered nuclides is written in Table 1. The decision of the usage of the 42 nuclide approximation was made based on the burnup credit isotopes [5] with consideration of  $^{135}$ Xe. The simulation of the xenon poisoning problematics was achieved by the elimination of  $^{135}$ I and  $^{135}$ Xe nuclei before the beginning of each cycle, i.e. K216, K217, K218, etc. This behaviour was assumed to be sufficient enough to simulate actual operational conditions in the LVR-15 reactor core.

Parameters for neutron population in criticality source mode of each individual Serpent calculation were set to 100 000 neutrons per generation, 200 active and 40 inactive generation cycles. Standard deviation of  $k_{\text{eff}}$  did not exceed 27 pcm for each calculation step. All Serpent calculations were carried out using the ENDF/B-VIII.0 [6] based cross section library.

## 4. Results

The collection of three entangled types of results is presented in this paper. The first type of results covers calculated atomic densities of chosen nuclide compared to the infinite lattice approximation. Second type of results represents verification of the calculated atomic densities with aim to determine whether the results are credible or not. The final part of the collection supports the statement that has been gained from the previous type of the results.

## 4.1. CALCULATED BURNUP QUALIFICATION

Visualization of <sup>239</sup>Pu atomic density burnup dependence has been chosen for the purpose of the calculated fuel burnup qualification. The axially averaged <sup>239</sup>Pu concentrations in the fuel as functions of burnup are provided in Figure 5. These results are taken from the advanced computational process described in Section 3. The visualization of the data is shown for all fuel assemblies with initial zero burnup at the moment of their first introduction into the LVR-15 reactor core during studied cycles K216–K229. The comparison with the infinite lattice calculated <sup>239</sup>Pu atomic densities is also included in Figure 5.



FIGURE 5. Axially averaged atomic densities of <sup>239</sup>Pu calculated for all fuel assemblies with initial zero burnup (left axis). The calculated values are compared with atomic densities from the infinite lattice approximation (right axis).



FIGURE 6. Comparison of assembly-wise atomic densities between the infinite lattice approximation and the unbroken burnup simulation of the opening step of the K216 cycle. Two fuel assemblies, standard 85A710 and control 65C666, has been taken into the account in the latter type of the calculation. Values for  $^{235}$ U,  $^{238}$ U,  $^{239}$ Pu and  $^{241}$ Pu are included.

A considerably profound discrepancies between the calculated results and the infinite lattice approximation can be observed in Figure 5. It is apparent that the amount of <sup>239</sup>Pu in case of the infinite lattice is one order of magnitude higher than in the results from the LVR-15 reactor operation history computation. The result of such kind raises the immediate demand for a validation of the entire computational process and for a verification of the data as well. The attempt to clarify these incompatibilities is the point of interest of the following type of the results collection.

#### 4.2. Computational process validation

The validation of the actual computational process has been carried out based on the previous results. Therefore, two kinds of problems have been compared. First, the burnup calculation of the infinite lattice approximation that was used as a prerequisite for the considered burnup library mentioned in Section 2. Second, an uninterrupted burnup calculation of the LVR-15 reactor core in the initial point of the whole computational process, i.e. the step 0 of the K216 cycle configuration.

This comparison also represents the difference in the non-leakage approach against the genuine core configuration calculation with emphasis on high heterogeneity and compactness of the LVR-15 core.

The data from the unbroken calculation of the opening step of the K216 cycle involves axially averaged atomic densities of the fresh standard and control fuel assemblies with identifiers 85A710 and 65C666, respectively.

Altogether, atomic density plots of 4 nuclides,  $^{235}$ U,  $^{238}$ U,  $^{239}$ Pu and  $^{241}$ Pu, are illustrated in Figure 6. The greatest similarity of the atomic density data is observable in case of  $^{235}$ U. Still, Figure 6 shows that the depletion of  $^{235}$ U is slightly more significant in case of both fuel assemblies from the unbroken cycle simulation. However, the differences for  $^{238}$ U and for both pictured isotopes of plutonium are more extensive. The production of plutonium is directly linked to the neutron capture on  $^{238}$ U nuclei. The Figure 6 indicates that there is a noticeably higher amount of  $^{238}$ U capture in the infinite lattice approximation and therefore a lesser concentration of the plutonium isotopes in the fuel assemblies of the comparison K216 cycle calculation.

To proceed to the main point of this validation analysis, there is a fundamental assumption that the <sup>239</sup>Pu atomic densities should be in the same order of magnitude as the atomic densities determined from the unbroken real core burnup calculation. Such accordance, however, has not been achieved. This outcome gives an evidence that some presumption in the designed computational process has been applied inaccurately. The investigation of the cause of the expressed discrepancies in the computational process is carried out in the following type of the results collection.

#### 4.3. The cause of discrepancies

The transfer of fuel composition data between particular steps of the computational process has been investigated as a potentially problematic part in the process design. More accurately, in the determination of which nuclides should be chosen for the conservation of atomic densities from one step to another.

Originally, there were 42 chosen nuclides as stated in Table 1. A new calculation concerning a first few steps of the carried out computational process was executed with the change in the number of chosen nuclides. This time, atomic densities of all nuclides in the Serpent cross section library from the end of a particular calculation step have been written into the input data of the following step. Due to this decision, the expected results have changed significantly



FIGURE 7. Short-term development of <sup>239</sup>Pu atomic densities for various calculation types.

towards the results that were observed in Figure 6. This behaviour for the case of  $^{239}$ Pu atomic densities is shown in Figure 7.

## **5.** DISCUSSION

According to the presented results, a misleading assumption in the design of the advanced computational process has been made. It has been investigated that the 42 nuclide representation does not reflect realistic conditions in the core during the LVR-15 reactor operation and thus a more comprehensive attitude has to be implemented. Clearly, the consideration of all nuclides available in the Serpent cross section library should be involved in the next generation of the LVR-15 reactor burnup computation.

Even though such upgrade of the computational process will require a larger amount of space for the output data storage, running time of the Serpent calculation of a single step will not be affected. This indicates the feasibility of the improvement.

On the other hand, the obtained results in Figure 5 shows the differences in the fuel composition based on the individual operation scheme of each fuel assembly. Therefore, the data can be used for analysis of the influence of the various schemes on the final form of the atomic density that will be represented in the burnup library of the LVR-15 reactor Serpent model.

## **6.** CONCLUSIONS

The Serpent computational model of the LVR-15 reactor has been introduced in this work with focus on the problematics of fuel burnup implementation. The advanced burnup computational process has been described using the most important aspects and operational characteristics of the LVR-15 reactor.

Currently available results have been presented and analyzed according to the additional calculations. The analysis has shown that the number of nuclides considered in the transfers between calculation steps have been chosen inaccurately. This misleading nuclide interpretation has caused significant discrepancies in the atomic density values between the computation and the fundamentally anticipated results from the infinite lattice approximation and from the unbroken burnup calculation of the realistic LVR-15 core.

The outcome of this paper will be used in the next generation of the advanced burnup computational process in order to determine a more realistic burnupwise fuel composition of the LVR-15 reactor.

#### LIST OF SYMBOLS

 $k_{\text{eff}}$  Effective multiplication factor

ENDF Evaluated Nuclear Data File

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