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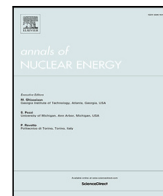
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# Development of a computational scheme based on the DRAGON5 code for the neutronic study of VVER-type reactor rods and assemblies

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## ABSTRACT

Open source modeling of VVER-type reactors could become a medium-term objective in Eastern Europe. As the deterministic code DRAGON5 could meet such a need, we confronted DRAGON5 against a stochastic reference code, SERPENT2. Our validation comprises 7 cells and 4 assemblies from the Khmelnytsky-2 reactor in Ukraine, within a wide range of heterogeneity levels in fuel composition. Two calculation schemes have been developed and compared. The first, the ALAMOS scheme, is highly discretized in energy and spatial resolution, while the second, the REL2005-like scheme, is calculated in two levels (one highly discretized in energy and the other highly discretized in space). In the majority of cases studied, both schemes offer satisfactory accuracy (e.g. less than 300 pcm in  $k_{\text{eff}}$ ), although there are difficulties related to energy deposition with gadolinium-poisoned fuel. While showing significantly poorer results than the ALAMOS scheme, the REL2005-like scheme offers lower computation times and major avenues for improvement remain to be explored. This work offers a first step towards the simulation of VVER-type reactors in DRAGON5, and paves the way for full-core simulations.

## 1. Introduction

The VVER-type reactors are currently the only commercial light water reactors in the world designed with hexagonal geometries for both pin cells and assemblies.

This Soviet and later Russian-designed reactor technology has been deployed in Russia and a number of Eastern European countries. Geopolitical tensions between Russia and VVER-equipped countries have prompted the latter to seek non-Russian simulation solutions. The European Union therefore decided to finance the CAMIVVER project (Verrier, 2024), coordinated by Framatome, with the aim of developing simulation and production calculation capabilities. In parallel with this project, and in cooperation with Framatome, Polytechnique Montréal wishes to offer an open-source solution based on the DRAGON5 code (Marleau et al., 2023).

Initial work on VVER modeling in DRAGON5 has been carried out in the article (Rooijen et al., 2017). More recently a team from the China Institute of Atomic Energy has produced important results for cells and assemblies modeling (Zhao et al., 2023). The aim of this work is to repeat and improve the results of this work but for the CAMIVVER reactors. The main indicators studied are the evolution of  $k_{\text{eff}}$ , isotopic concentrations and some reaction rates. The results obtained with DRAGON5 were compared with those of a stochastic

reference code, SERPENT2 (Leppänen et al., 2015). Here we present the results obtained for the cells and assemblies of the Khmelnytsky-2 reactor, which is highly heterogeneous in its composition. A side objective of this work is to compare two hexagonal assembly modeling schemes in DRAGON5. Based on the ALAMOS platform, the first, the ALAMOS scheme, is a classic single-level scheme (direct scheme). The ALAMOS platform is external to DRAGON5 and provides geometries that can be used by DRAGON5 in place of native geometries. The second, the REL2005-like scheme, is a two-level scheme based on the one presented in Vidal et al. (2007). The structure of these schemes will be detailed in Section 2.2.

## 2. Study cases and calculation schemes

First, we present the characteristics of the cells and assemblies studied (geometries and composition). Data concerning the compositions and geometries of the various cells and assemblies come from the public CAMIVVER project data available in the report (Willien and Vezzoni, 2021). Secondly, we present the structure of our calculation schemes. The detailed software architecture of the scripts (Python encapsulation) is available in Fede and François (2023).

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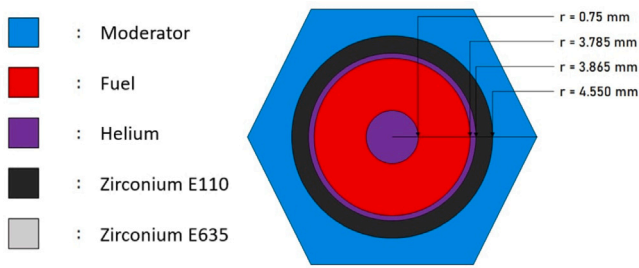


Fig. 1. Cell geometry. The figure shows the different crowns of the cell with their radii. The compositions are shown on the left.

**Table 1**  
Isotopic composition of fuel in each cell.

Cell names	Assemblies	<sup>235</sup> U Enrichment	w% Gd <sub>2</sub> O <sub>3</sub>
22AU_22UOx	22AU	2.2%	∅
40AU_40UOx	40AU	4.0%	∅
439GT_44UOx	439GT	4.4%	∅
439GT_36Gd		3.6%	5.0%
39AWU_40UOx (398GO_40UOx)	39AWU	4.0%	∅
39AWU_36UOx		3.6%	∅
39AWU_33Gd (398GO_33Gd)		3.3%	5.0%

**Table 2**  
Number of fuel rods of each type per assembly (total: 312).

	22AU	40AU	398GO	39AWU
22AU_22UOx	312			
40AU_40UOx		312		
398GO_40UOx			306	
398GO_33Gd			6	
39AWU_40UOx				252
39AWU_36UOx				51
39AWU_33Gd				9

## 2.1. Studied geometries and compositions

We have chosen to focus on 7 cells from the Khmel'nitsky-2 reactor, from 4 different assemblies. Fig. 1 shows the dimensions of the 7 cells, while Table 1 presents the main information concerning the compositions of the different cells. Further details can be obtained by consulting (Willien and Vezzoni, 2021).

As far as assemblies are concerned, we decided to study 4 assemblies covering a wide range of enrichment and heterogeneity. In addition to fuel cells, the assemblies include guide tubes and stiffeners. Each assembly includes 312 fuel rods, 18 guide tubes and a central guide tube bringing the total assembly to 331 elements. The pitch of the assemblies is 23.6 cm. Table 2 describes the type and number of rods present in the various assemblies. Fig. 3 describes the arrangement of the different types of fuel rods in assemblies 22AU and 40AU, 439GT and 39AWU.

Guide tubes and stiffeners are made from E635 zirconium alloy. The guide tubes (respectively center tubes) are modeled as hollow tubes with inner radii of 5.450 mm (resp. 5.350 mm) and outer radii of 6.300 mm (resp. 6.374 mm). The geometric characteristics of stiffeners are shown in Fig. 2. A gap of 1.2 mm is present between the stiffeners of two assemblies.

**Remark 1.** The 439GT assembly has not been processed, but it is described here as results were obtained on the cells making it up.

**Remark 2.** Note that the 40AU\_40UOx cell and 40AU assembly are not directly derived from the CAMIVVER project, but are our own

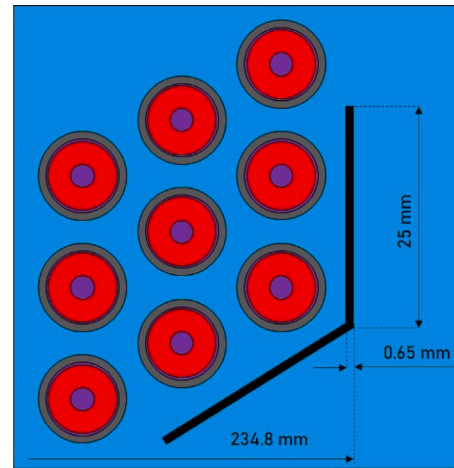


Fig. 2. Stiffener geometry. The figure shows the main geometric characteristics of the stiffeners.

variations of the 22AU\_22UOx cell and 22AU assembly in order to create an intermediate assembly between the 22AU and 398GO assemblies.

## 2.2. Calculation schemes

Optimization studies of the parameters of the various modules have been carried out and are presented in the reports (Richard, 2023) for DRAGON5 and (Fede and François, 2023) for SERPENT2. Key points include the fact that cells are discretized into 4 or 6 fuel rings, respectively without and with gadolinium in the initial fuel composition (for DRAGON5 and SERPENT2), with the exception of gadolinium cells in ALAMOS geometries which have 11 rings. It should also be noted that for SERPENT2, 500 populations of 16,000 neutrons have been used in the calculations.

Assemblies 22AU, 40AU and 398GO have 60° rotational symmetry, while assembly 39AWU has 120° rotational symmetry. So only one-sixth (22AU, 40AU and 398GO) or one-third (39AWU) of the assemblies have been modeled and are shown below.

The presence of stiffeners increases the complexity of the assembly modeling. DRAGON5 does not allow stiffeners to be modeled natively on hexagonal geometries. However, DRAGON5 is able to handle externally modeled geometries with stiffeners. This is the approach we choose to develop the ALAMOS calculation scheme. The geometries generated by the ALAMOS platform (and all data sets) are available in the archives of the Institut de Génie Nucléaire (Fede and François, 2023). We remind that technical informations about the ALAMOS platform can be found in Tomatis et al. (2022).

All calculations (including those performed with SERPENT2) are performed using libraries generated from the JEFF-3.1.1 nuclear data library. The libraries used, and generated using NJOY (Zu et al., 2023), are energy-continuous in ACE format for SERPENT2, and multi-group in Draglib format for DRAGON5.

### 2.2.1. ALAMOS scheme

The ALAMOS scheme is a direct scheme. Its diagram is shown in Fig. 4. Two tracking steps are performed. The first with the SALT: module for self-shielding, and the second with the SYBILT: and MCCGT: modules for flux calculation using the characteristic method. Due to cell numbering in the ALAMOS files, we have to use the same geometry for both calculations, although the scheme we have developed theoretically allows us to distinguish two different geometries. A non-sectorized geometry has been chosen to keep calculation times acceptable. For energy discretization, a library of 295 groups was chosen on the basis of the article (Hébert, 2009).

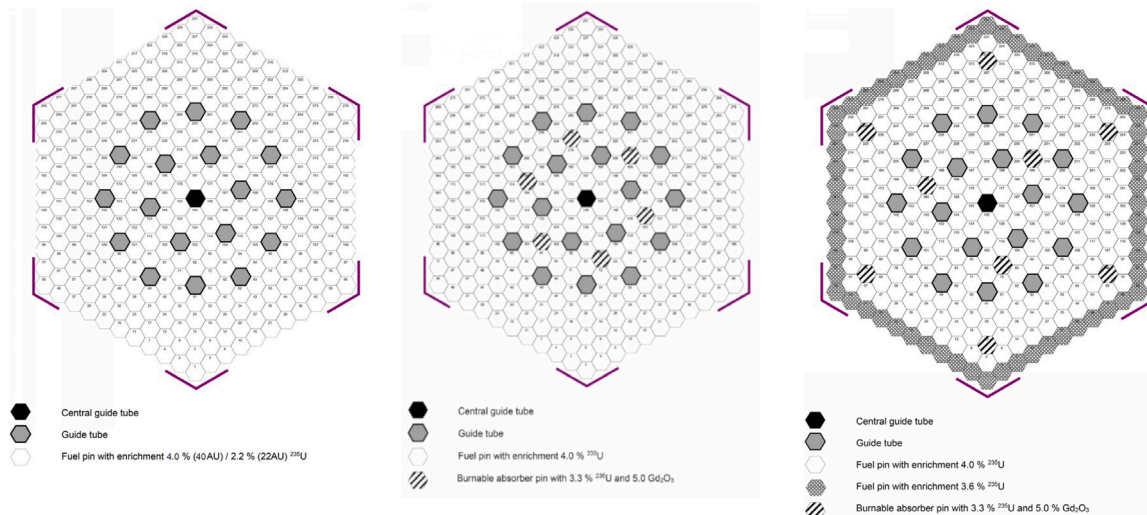


Fig. 3. Cell layout for studied assemblies, from Willien and Vezzoni (2021). From left to right, the different arrangements of assemblies 22AU (analog to 40AU), 398GO and 39AWU are shown. Guide and center tubes are shown in uniform dark gray and black. Cells with gadolinium are shown in hatched gray. And on the outer rim of the 39AWU assembly (right), cells with lower enrichment are dotted.

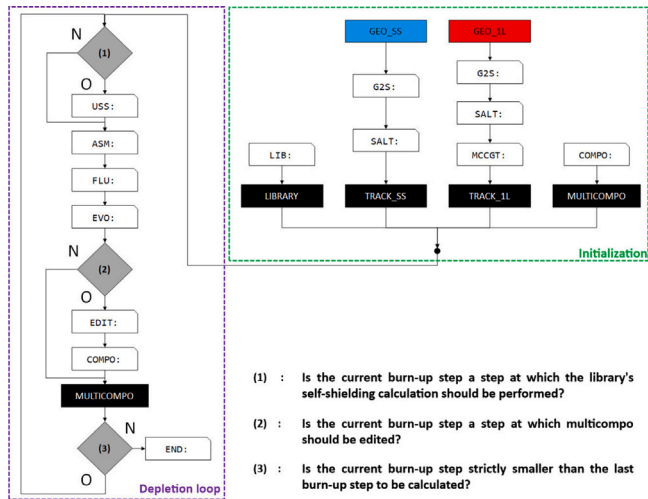


Fig. 4. ALAMOS calculation scheme. The calculation scheme is described in two steps. On the top right, the initialization section, with descriptions of geometries, isotopic compositions, definition of effective cross-section libraries and calculation of various tracking parameters. On the left are the evolving calculation loops, with the various loop stopping criteria at bottom right.

### 2.2.2. REL2005-like scheme

Inspired by the REL2005 scheme developed in the article (Vidal et al., 2007), we have developed a second calculation scheme called REL2005-like. Its diagram is shown in Fig. 5. Our aim is to achieve lower computation times and to work with sectorization around the fuel cells. The special feature of this scheme is that it has two levels of flux calculation. In the first level, the flux is calculated with a high energy discretization (295 groups) but a low spatial discretization. The geometry of this level is native to DRAGON5, and the current interface collision probability method is used to calculate the flux for fast calculation times. The second level is strongly spatially discretized and weakly energy-discretized, with only 26 energy groups. The geometry used is the ALAMOS geometry, the most highly discretized possible, and the flux calculation method used is the characteristic method. As mentioned previously, stiffeners are only taken into account in ALAMOS geometries, i.e. only on the second level here.

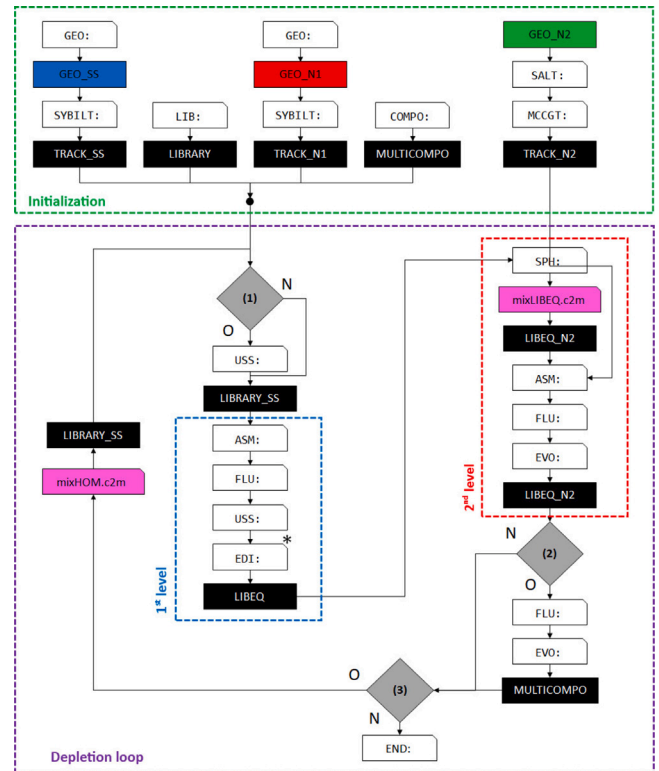


Fig. 5. REL2005-like calculation scheme. This diagram has the same structure as the ALAMOS diagram, with initialization at the top and calculation in progress at the bottom. The main difference is the presence of two levels based on two different geometries in the depletion loop. The criteria for stopping loops are identical to those in Fig. 4.

### 2.2.3. Calculation scheme for an isolated cell

The calculation scheme used for a cell alone (i.e. not in a full assembly) is similar to the ALAMOS scheme presented above in Section 2.2.1 and in Fig. 4. The main difference is that an isolated cell has its geometry natively coded in DRAGON5 (whereas ALAMOS geometries, used for full assemblies, are imported data). Please refer to the report (Fede and Francois, 2023) for more details.

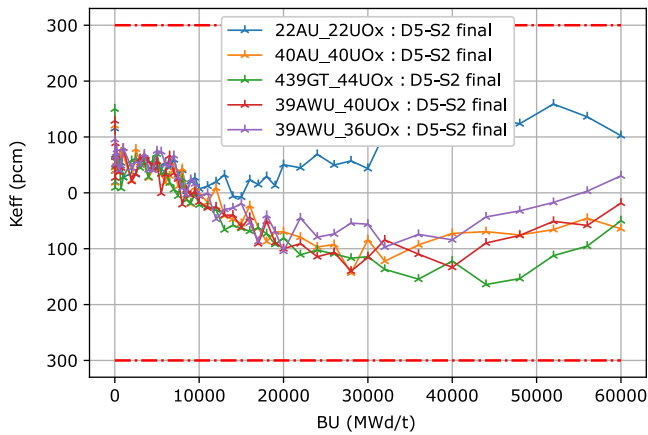


Fig. 6. Evolution of DRAGON5-SERPENT2 discrepancy on  $k_{\text{eff}}$  in gadolinium-free cells. For all cells without gadolinium, the  $k_{\text{eff}}$  discrepancy remained low and stable at less than 300 pcm.

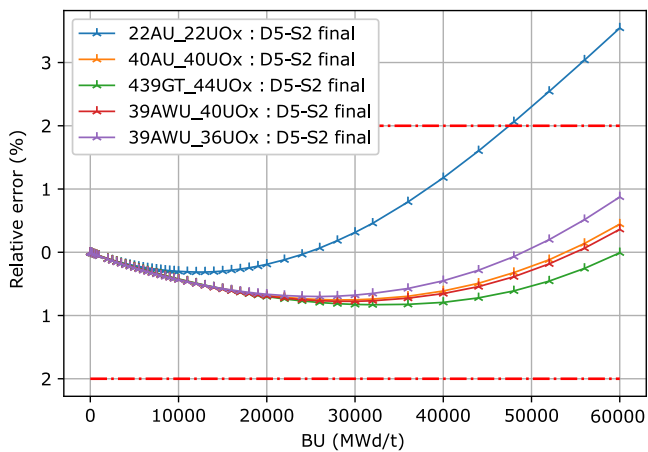


Fig. 7. Evolution of the DRAGON5-SERPENT2 discrepancy in  $^{235}\text{U}$  mass concentration in gadolinium-free cells. With the exception of the least highly enriched cell (22AU\_22UOx), the discrepancy in mass concentrations does not exceed 2% for gadolinium-free cells.

### 3. Numerical results

The most notable results are listed here. We will focus on the evolution of DRAGON5-SERPENT2 discrepancy in  $k_{\text{eff}}$  and mass concentrations of particular isotopes. We will briefly mention some reaction rates. Full results can be found in the archives of the Institut de Génie Nucléaire website (Fede and François, 2023).

#### 3.1. Cells without gadolinium in initial composition

Figs. 6–8 show the evolution of DRAGON5-SERPENT2 discrepancy on gadolinium-free cells alone. These results are fairly typical of our own: the discrepancies are satisfactory (less than 300 pcm for  $k_{\text{eff}}$  and less than 2% deviation for isotopic concentrations) except on cells weakly enriched for a few isotopes:  $^{235}\text{U}$ ,  $^{155}\text{Gd}$  and  $^{157}\text{Gd}$ , whose isotopic concentrations show discrepancies of up to 6.0%.

#### 3.2. Cells with gadolinium in initial composition

These difficulties in accurately calculating gadolinium isotope concentrations are exacerbated for cells initially containing a high proportion of gadolinium. The preceding quantities have been determined also for cells with gadolinium and are presented in Figs. 9–11. The presence

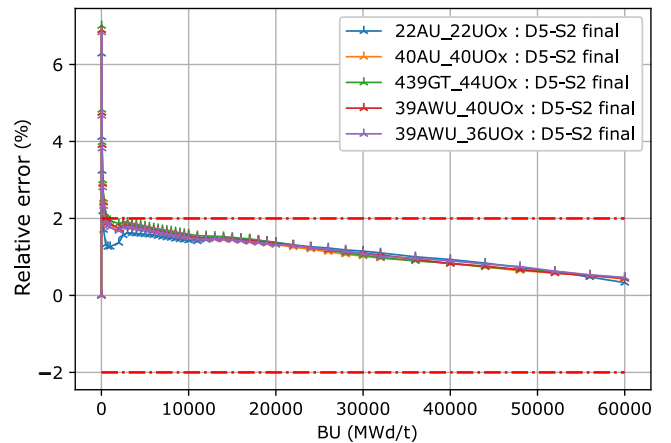


Fig. 8. Evolution of the DRAGON5-SERPENT2 discrepancy in  $^{239}\text{Pu}$  mass concentration in gadolinium-free cells. With the exception of an initial peak the discrepancy in mass concentrations does not exceed 2% for gadolinium-free cells.

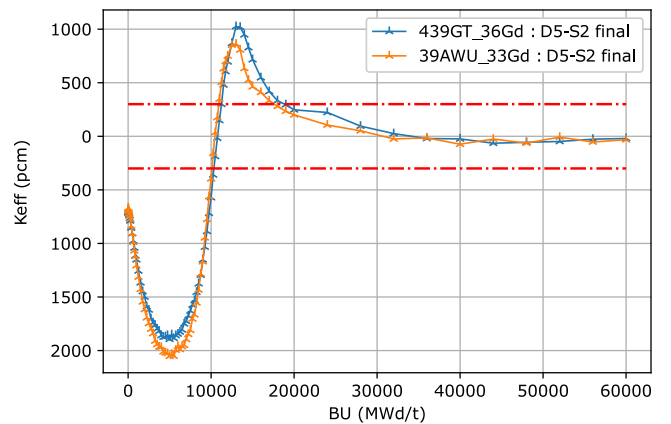


Fig. 9. Evolution of DRAGON5-SERPENT2 discrepancy on  $k_{\text{eff}}$  in cells with gadolinium. As long as the initial gadolinium has not been consumed ( $<20 \text{ Gwd t}^{-1}$ ) DRAGON5 discrepancies are high; then the situation regularizes at the end of the depletion.

of gadolinium is known to make numerical calculations difficult. Only the concentrations of  $^{235}\text{U}$  and  $^{238}\text{U}$  show a small discrepancy ( $<2\%$ ) between DRAGON5 and SERPENT2 over the whole depletion for both cells with gadolinium while others, such as  $^{239}\text{Pu}$ , show significant deviations until the gadolinium has been completely consumed.

We will discuss our possible solutions to reduce discrepancies in Section 4. However, we can mention the fact that these cells are highly subcritical and are therefore always associated with other cells in assemblies. We can therefore hope that their small number in an assembly will enable us to obtain interesting results on the scale of assemblies.

#### 3.3. Assemblies without gadolinium in initial composition

The results obtained for gadolinium-free assemblies are very similar to those obtained for constitutive cells. Fig. 12 shows the results obtained on  $k_{\text{eff}}$ . It can be seen that the REL2005-like scheme is in better agreement at low enrichment (and therefore low reactivity), while the ALAMOS scheme is more accurate at more conventional enrichment (4%). Discrepancies in isotopic concentrations are similar to those obtained for single cells. Fig. 13 shows these discrepancies for  $^{239}\text{Pu}$ . Note that the ALAMOS scheme gives slightly better results than the REL2005-like scheme.

Figs. 14 and 15 show, respectively for the ALAMOS scheme and the REL2005-like scheme, fission rates in the thermal domain at the

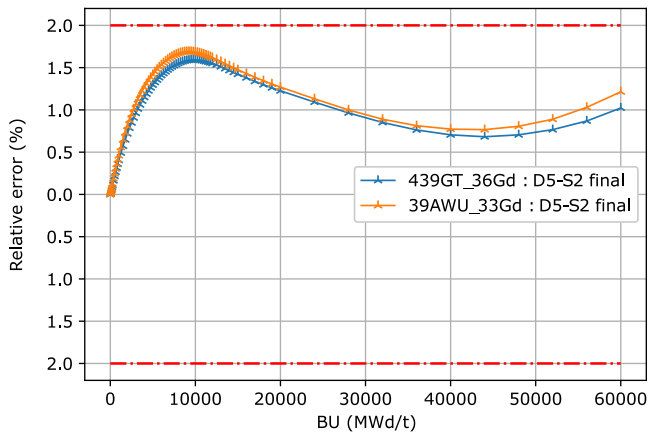


Fig. 10. Evolution of the DRAGON5-SERPENT2 discrepancy in  $^{235}\text{U}$  in cells with gadolinium. Some isotopes, such as  $^{235}\text{U}$  here, have their concentrations determined with little discrepancy compared to SERPENT2.

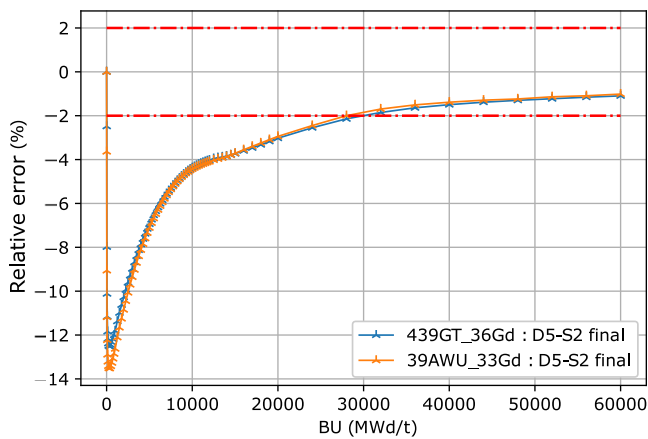


Fig. 11. Evolution of the DRAGON5-SERPENT2 discrepancy in  $^{239}\text{Pu}$  in cells with gadolinium. Other isotopes, such as  $^{239}\text{Pu}$  here, have their concentrations determined with discrepancy compared to SERPENT2 until the gadolinium has been completely consumed.

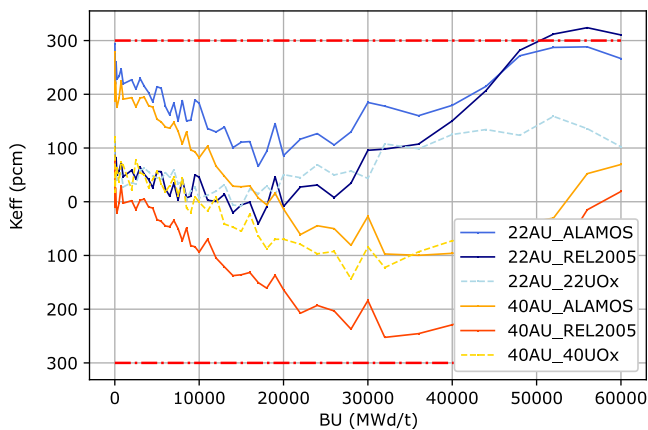


Fig. 12. Evolution of DRAGON5-SERPENT2 discrepancy on  $k_{\text{eff}}$  in 22AU and 40AU assemblies. The dotted line shows our results for the constituent cells of the two assemblies, 22AU\_22UOx and 40AU\_40UOx respectively. Discrepancies are slightly higher for assemblies than for cells, but remain around 300 pcm.

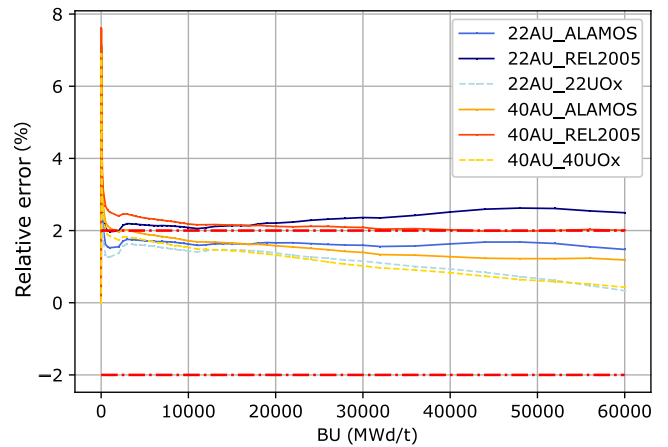


Fig. 13. Evolution of the DRAGON5-SERPENT2 discrepancy in  $^{239}\text{Pu}$  in 22AU and 40AU assemblies. The dotted line shows our results for the constituent cells of the two assemblies, 22AU\_22UOx and 40AU\_40UOx respectively.

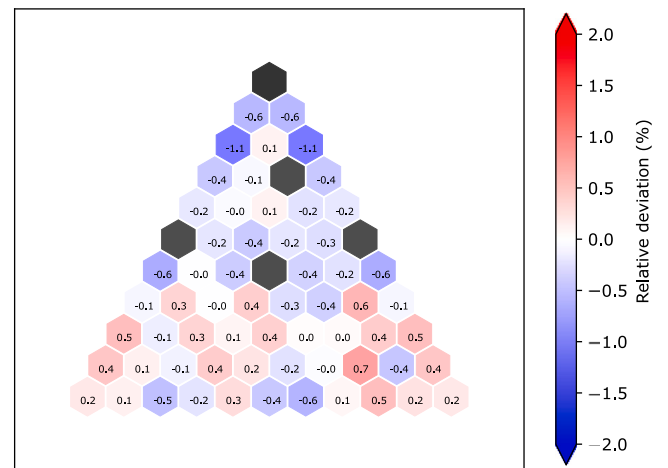


Fig. 14. 40AU assembly DRAGON5-SERPENT2 relative difference in neutron flux for thermal neutrons at the end of depletion ( $60 \text{ GWd t}^{-1}$ ) determined by the ALAMOS calculation scheme.

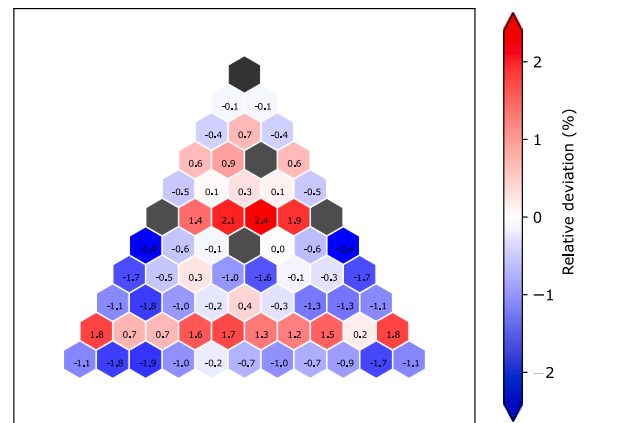


Fig. 15. 40AU assembly DRAGON5-SERPENT2 relative difference in neutron flux layer for thermal neutrons at the end of depletion ( $60 \text{ GWd t}^{-1}$ ) determined by the REL2005-like calculation scheme.

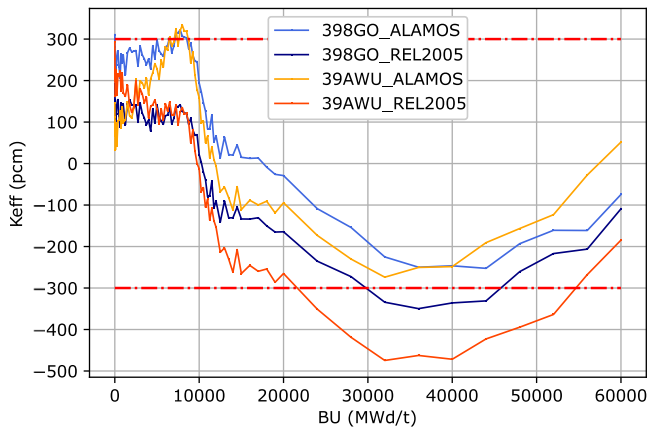


Fig. 16. Evolution of DRAGON5-SERPENT2 discrepancy on  $k_{eff}$  in 398GO and 39AWU assemblies. The REL2005-like scheme has maximum discrepancies of between 300 and 500 pcm, while the ALAMOS scheme has discrepancies of less than 300 pcm.

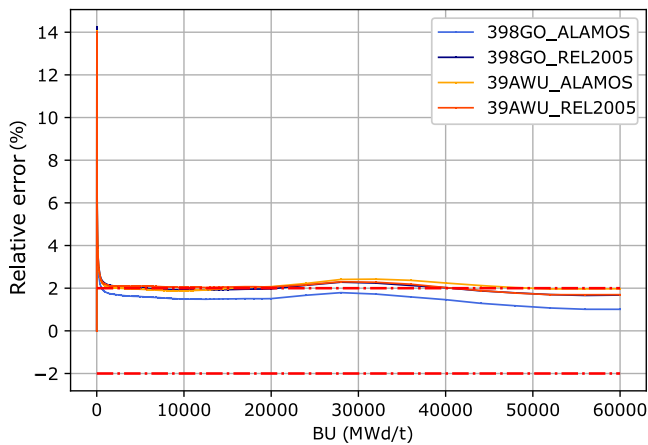


Fig. 17. Evolution of the DRAGON5-SERPENT2 discrepancy in  $^{239}\text{Pu}$  in 398GO and 39AWU assemblies.

end of depletion ( $60 \text{ GWd t}^{-1}$ ) for the 40AU assembly. Similar discrepancy levels are observed. However, the discrepancies are relatively homogeneous, with an order of magnitude of 1%–2%.

### 3.4. Assemblies with gadolinium in initial composition

Fig. 16 shows the  $k_{eff}$  discrepancies for the 39AWU and 398GO assemblies. The ALAMOS pattern shows results significantly in better agreement than the REL2005-like pattern, with deviations from the reference less than 300 pcm versus 300 to 500 pcm for the REL2005-like pattern in the middle of depletion. Because of the low number of cells with gadolinium in their initial composition, the results obtained for isotopic evolutions are close to those for cells without gadolinium, as expected. Fig. 17 shows the example of  $^{239}\text{Pu}$ , where the DRAGON5-SERPENT2 discrepancy has the same appearance as in Fig. 8 (gadolinium-free cells) and 13 (gadolinium-free assemblies).

**Remark 3.** The assemblies here are made up of several cell types (Table 2) and it is therefore not possible to directly compare these results with those obtained at cell scale.

Figs. 18 and 19 show, respectively for the ALAMOS scheme and the REL2005-like scheme, fission rates in the thermal domain at the end of depletion ( $60 \text{ GWd t}^{-1}$ ) for the 398GO assembly. We can clearly see that the cell with gadolinium is in poor agreement, with discrepancies of the order of 4% for both schemes. The other cells are simulated with

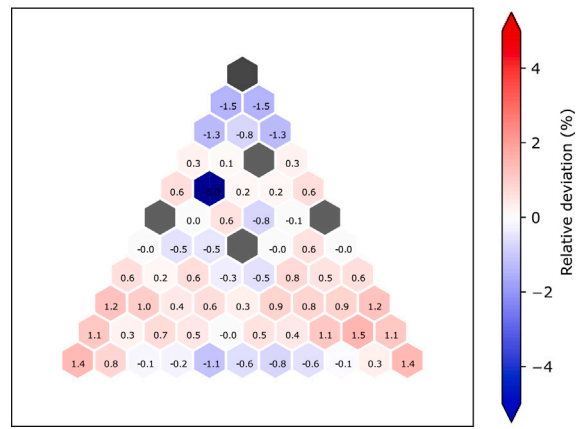


Fig. 18. 398GO assembly DRAGON5-SERPENT2 relative difference in neutron flux layer for thermal neutrons at the end of depletion ( $60 \text{ GWd t}^{-1}$ ) determined by the ALAMOS calculation scheme.

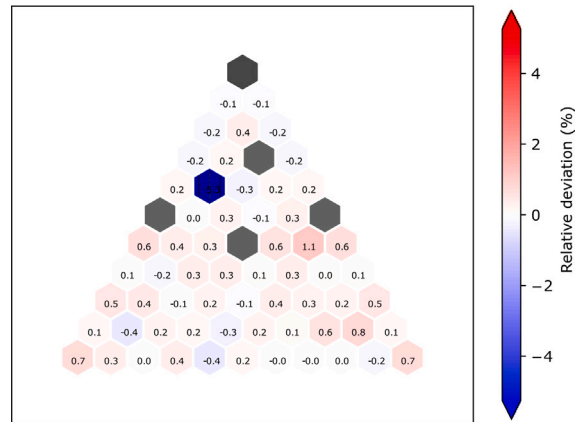


Fig. 19. 398GO assembly DRAGON5-SERPENT2 relative difference in neutron flux layer for thermal neutrons at the end of depletion ( $60 \text{ GWd t}^{-1}$ ) determined by the REL2005-like calculation scheme.

discrepancies of less than 2% for both schemes. These figures also show that for the REL2005-like scheme, there are larger discrepancies on the assembly boundaries than the ALAMOS scheme. This may be due to the partial inclusion of stiffeners in the REL2005-like scheme. It is, however, difficult to identify the discrepancies due to stiffeners from those of other sources.

### 3.5. Summary

Table 4 summarizes the different results obtained for global quantities ( $k_{eff}$  and isotopic concentrations averaged over assemblies) by the two ALAMOS and REL2005-like schemes on the four assemblies 22AU, 40AU, 398GO and 39AWU. The results obtained with the ALAMOS scheme are similar to those obtained with SERPENT2, particularly in terms of  $k_{eff}$  and concentrations of the main radioactive isotopes. A large amount of gadolinium slightly increases discrepancies between DRAGON5 and SERPENT2, particularly when assessing the concentrations of elements produced by gadolinium decay. The REL2005-like scheme shows larger discrepancies, particularly in the presence of gadolinium.

Reaction rates deviations from the SERPENT2 reference are shown in Table 5. As with the global quantities, the ALAMOS scheme offers lower discrepancies than the REL2005-like scheme, and assemblies containing gadolinium show greater deviations from the reference. Average of mean deviations are lower than 1%, while average of

**Table 3**  
Synthesis of average computation times (in hours).

	ALAMOS	REL2005-like	Gain in computation times
Gd free assemblies	80.4	63.7	≈21%
Gd assemblies	152.2	118.5	≈22%

**Table 4**  
Synthesis of mean global quantities for assembly calculations. The right-hand side of the table corresponds to the 11 isotopes we have focused on:  $^{235}\text{U}$ ,  $^{236}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ ,  $^{242}\text{Pu}$ ,  $^{155}\text{Gd}$ ,  $^{157}\text{Gd}$ ,  $^{149}\text{Sm}$  and  $^{135}\text{Xe}$ .

	$\Delta k_{eff} < 300$ pcm		$\Delta N_i < 2\%$	
	ALAMOS	REL2005-like	ALAMOS	REL2005-like
Gd free assemblies	v	v	8/11	5/11
Gd assemblies	v	x	6/11	6/11

maximum deviations reaches ~2% for assemblies without gadolinium and ~4% for assemblies with gadolinium. The REL2005-like scheme shows greater deviations from SERPENT2 than the ALAMOS scheme. It should be noted, however, that local quantities, when averaged over the assembly, show low deviations in all situations (ALAMOS/REL2005-like and with/without gadolinium).

Finally, in terms of calculation times, we observe in Table 3 a 21% or 22% gain when using the REL2005 scheme rather than the ALAMOS scheme, respectively without or with gadolinium in the initial composition.

## 4. Discussion

### 4.1. Quality of results

Overall, the results are quite good. The orders of magnitude are generally within the limits we expected (of the order of 300 pcm for the  $k_{eff}$  and 2% for the other quantities). Quite extensive parametric optimization work has been carried out (see the report Richard, 2023), enabling us to ensure the consistency of the results obtained. However, the results for the REL2005-like scheme are limited: as expected, this scheme brings a significant reduction in computation times, but also a significant increase in discrepancies compared with the ALAMOS scheme, which is slower but more reliable. Finally, it should be noted that the simulation of cells with gadolinium and therefore low initial reactivity are very poorly modeled by DRAGON5. Several avenues have been explored to reduce discrepancies (notably by working on the calculation of cross-sections self-shielding), but none has been fully successful yet.

### 4.2. Areas for improvement

We have identified several ways of further improving our simulations.

- As mentioned previously, parametric optimization at the cell scale was crucial in obtaining satisfactory results. This work was partially carried out at assembly scale, but the performance limitations of our computing servers prevented us from going into as much detail as we would have liked.

- At this point, it is not possible to natively implement stiffeners in hexagonal geometry, which has led to a degradation in the performance of the REL2005-like scheme. Taking stiffeners into account by integrating their composition into the moderator of adjacent cells at the first level of the REL2005-like scheme could lead to significant improvements in accuracy. In addition, the revision of certain numerical simplification assumptions could further improve the accuracy of the REL2005-like scheme, notably the revision of cell families for the interface current method.
- A final major area for improvement is the revision of energy deposition models (Tuominen et al., 2019). We discovered that energy deposition with SERPENT2 is not correctly handled with the legacy JEFF-3.1.1 libraries distributed with the code. Improved SERPENT2 libraries with the edpmode=2 flag have been processed by Vivian Salino in Salino (2023), but too late to be used in this study. New Serpent libraries have an influence far greater than the statistical uncertainties obtained from our SERPENT2 simulations.

## 5. Conclusion

The results obtained in this work have established DRAGON5's ability to model hexagonal cells and assemblies for VVER-type reactors. Two calculation schemes have been developed with a view to industrial use. The deviations obtained with the SERPENT2 reference code demonstrate the possibility of achieving sufficient accuracy for operational calculations. Although adjustments are still needed to improve the calculation schemes, in particular the REL2005-like scheme, the quality of assembly simulation with the DRAGON5 code is sufficient to consider full-core simulation with the associated DONJON5 code.

### CRedit authorship contribution statement

**Cyprien Richard:** Methodology, Software, Validation, Formal analysis, Investigation, Writing – original Draft, Writing – review & editing, Visualization. **Mathias François:** Methodology, Software, Validation, Formal analysis, Investigation, Writing – review & editing, Visualization. **Lucas Fede:** Methodology, Software, Validation, Formal analysis, Investigation, Writing – review & editing, Visualization. **Alain Hébert:** Conceptualization, Methodology, Software, Validation, Resources, Data curation, Writing – review & editing, Supervision, Project administration.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

### Data availability

The data are freely available online at the addresses given in the references.

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**Table 5**  
Synthesis of local quantities (reaction rates) for assembly calculations. Mean deviations are obtained by  $\sum_{cells} |deviation|_{S2-D5} / N_{cells}$ .

	Average of mean deviations (%)		Average of max. deviation (%)	
	ALAMOS	REL2005-like	ALAMOS	REL2005-like
Gd free assemblies	0.64	0.88	1.41	2.31
Gd assemblies	0.79	0.84	3.08	4.07



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