Monte-Carlo Coupled Depletion Codes Efficiency for Research Reactor Design

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Abstract. In the field of industrial studies, burnup calculations and associated neutronic parameters are most often determined using deterministic methods. Even though they are faster than Monte-Carlo methods and efficient concerning the determination of best estimate physical quantities, they however have drawbacks: these tools rely on certain conditions and reactor characteristics (such as energetic spectrum, lattice pattern, types of fuel, etc.) and are based on neutronic assumptions and numerical approximations. On the other hand, Monte-Carlo methods are not problem-dependent. They do not require approximations, all kinds of complex geometries can be modelled and the whole interaction processes can be treated with the best state-of-the-art knowledge. Due to flexibility and accuracy, Monte-Carlo burnup calculations are frequently used in R&D studies, where faster deterministic burnup calculations are more suitable for industrial studies (best cost/accuracy ratio). With the improvement of CPU power, Monte-Carlo codes ability for burnup calculation has to be tested in order to determine whether their performances are convenient for industrial studies. This paper proposes to perform a comparison between Monte-Carlo codes used by TechnicAtome (TRIPOLI-4® [1], MCNP6 [2] and Serpent [3]) and the deterministic scheme COCONEUT [4]. This comparison also provides the Validation and Verification process (V&V) undergone by COCONEUT [5]. This is carried out on standard fuel assembly (SFA), absorber fuel assembly (AFA) of a core with burnable poison and on the full 2D core. Such geometry is used by TechnicAtome to set new methodology studies. Parameters such as reactivity, isotope concentration and neutronic flux are studied on a burn-up calculation reaching around 100 GWd/tU per assembly. Excellent agreement is observed between all codes.

1. Introduction

Early stages of core design and industrial studies require a quick and efficient calculation of key neutronic parameters (reactivity, control rods efficiency, power peak factors, core material balance, etc.) at any given step during core cycle. This determination is mainly achieved by deterministic calculation schemes and TechnicAtome has developed its own tool named COCONEUT[1] (COre COnception NEUtronic Tool) dedicated to research reactor calculation. The aim of this tool - based on deterministic codes APOLLO2 [6] (2D, multigroup transport theory) and CRONOS2 [7] (3D, diffusion theory) – is to be generic and to perform accurate calculations of MTR-type reactors with limited CPU-time.

Improvement of CPU power allows considering Monte-Carlo burnup calculations for industrial studies. This paper proposes to perform a comparison between Monte-Carlo codes commonly used by TechnicAtome (TRIPOLI-4®, MCNP6 and Serpent) with COCONEUT. The aim is twofold:

- Determine whether Monte-Carlo codes performances are convenient in case of burnup calculation for industrial studies.
- Describe the Validation and Verification (V&V) process undergone by COCONEUT.

This is carried out on standard fuel assembly (SFA), absorber fuel assembly (AFA) of a core with burnable poison and on the full 2D core. Such geometries are used by TechnicAtome to

[1] Neutronic codes are written with capital letters in this paper

set new methodology studies. Parameters such as reactivity, isotopes concentration of interest and neutronic flux are studied on a burn-up calculation reaching 100 GWd/tU.

The deterministic codes have advantages of fast execution and acceptable accuracy if the appropriate modeling features are used. It is very important to estimate accurately the burnup dependent behavior of research reactors, for the best operation of the reactor, safety analysis and the establishment of strategic planning for fuel management. However, for a three-level calculation (cell transport calculation, assembly transport calculation and full core diffusion calculation), careful modifications have to be made in order to simulate accurately the neutronic behavior of the research reactors using full core diffusion calculation.

2. Description of the Study Cases

2.1 Model overview

The study case is a dummy core [8] design by TechnicAtome for frequent and intensive verification and validation processes. Several loading patterns of the non-existent core are studied at TechnicAtome according to the needs of the neutronic research team. The case considered here is loaded with 32 fuel assemblies, as shown in FIG. 1 (16 standard fuel assemblies and 16 hafnium-plate controlled assemblies).

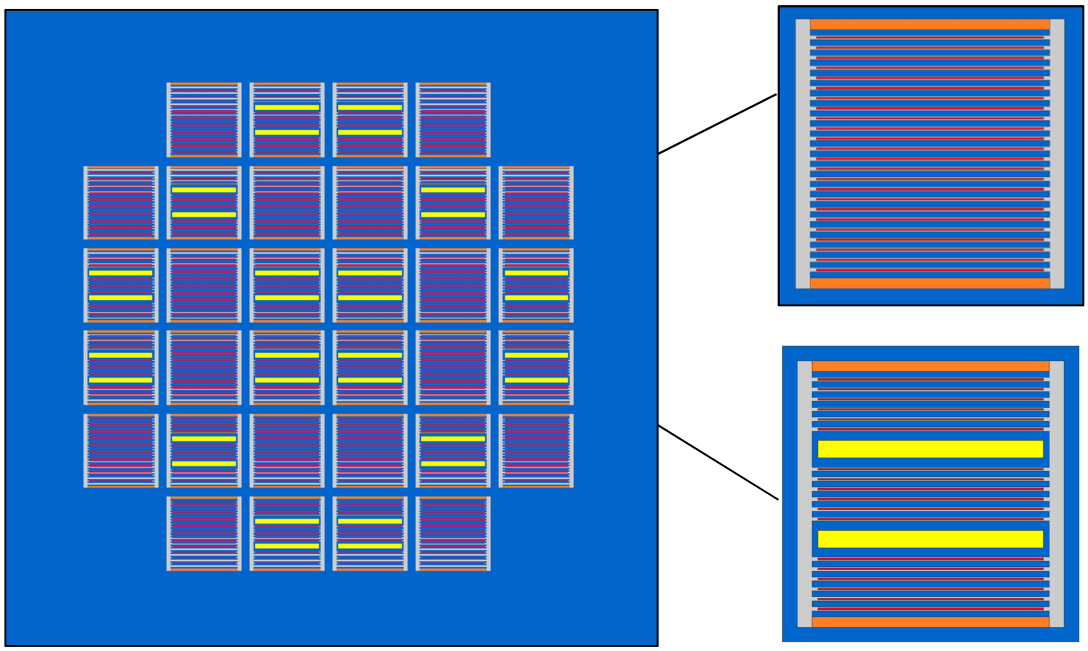

FIG. 1. Dummy core design by TechnicAtome for validation process (hafnium plate: yellow ; natural boron: orange).

The standard fuel assembly (SFA) is made of 24 fuel plates while the absorber fuel assembly (AFA) only contains 18 plates. The 6 removed plates are replaced by two hafnium control rods, 6 mm wide. A U_3-Si_2 dispersed fresh fuel is considered within this study. Natural boron is placed as a burnable poison in the external part of the aluminum rack to control the exceeding reactivity. The full dimensions of both assemblies are identical and are 9 x 9 cm in xy plan, and the active part is 80 cm high. Furthermore, the fuel array grid is identical in both fuel assemblies.

2.2 Benchmark considerations

The same consistent parameters are taken into account for each code and simulation:

- JEFF-3.1.1 nuclear data library [9];
- 50 burnup steps with a maximum value of 100 GWd/tU. These steps are chosen to take into account Xe buildup and boron consumption;
- Core power of 50 MWth and mean assembly power of 1.5625 MWth;
- Geometry, initial composition and temperature (300 K for each medium);
- Depletion in fuel plates and in material with burnable poison only;
- Unresolved resonance range treatment;
- Depletion chain (as close as possible);
- Default biasing techniques (no analog).

In the particular case of 2D lattice calculations:

- Reflecting surface are defined as boundary conditions on outer limits.

Main hypotheses and methods for each code are discussed in the next two sections.

3. Deterministic Depletion Calculation Code

3.1 General Features of COCONEUT

TechnicAtome neutronic calculation tool for Research Reactors core design and optimization, named COCONEUT, allows performing equilibrium core depletion and neutronic analysis on complex geometries. COCONEUT comprises deterministic calculation scheme and stochastic reference calculation line. The deterministic scheme is mainly used for core equilibrium states assessment and to export the fuel assembly burnup compositions to Monte Carlo codes. Deterministic calculations are performed on both multigroup transport (2D) theory and diffusion theory (3D) using APOLLO2 and CRONOS2 CEA codes. An overview of the COCONEUT different calculation steps is presented in FIG. 2.

COCONEUT is currently undergoing a large validation and qualification process on its latest released version. Biases and uncertainties are easily assessed by comparisons with Monte Carlo simulation for fresh fuel. Depleted configurations use deterministic calculation material balance as an input and are compared to full stochastic calculations. It is planned as part of the validation process to estimate the impact of deterministic main assumptions on depleted composition with Monte Carlo burn-up codes.

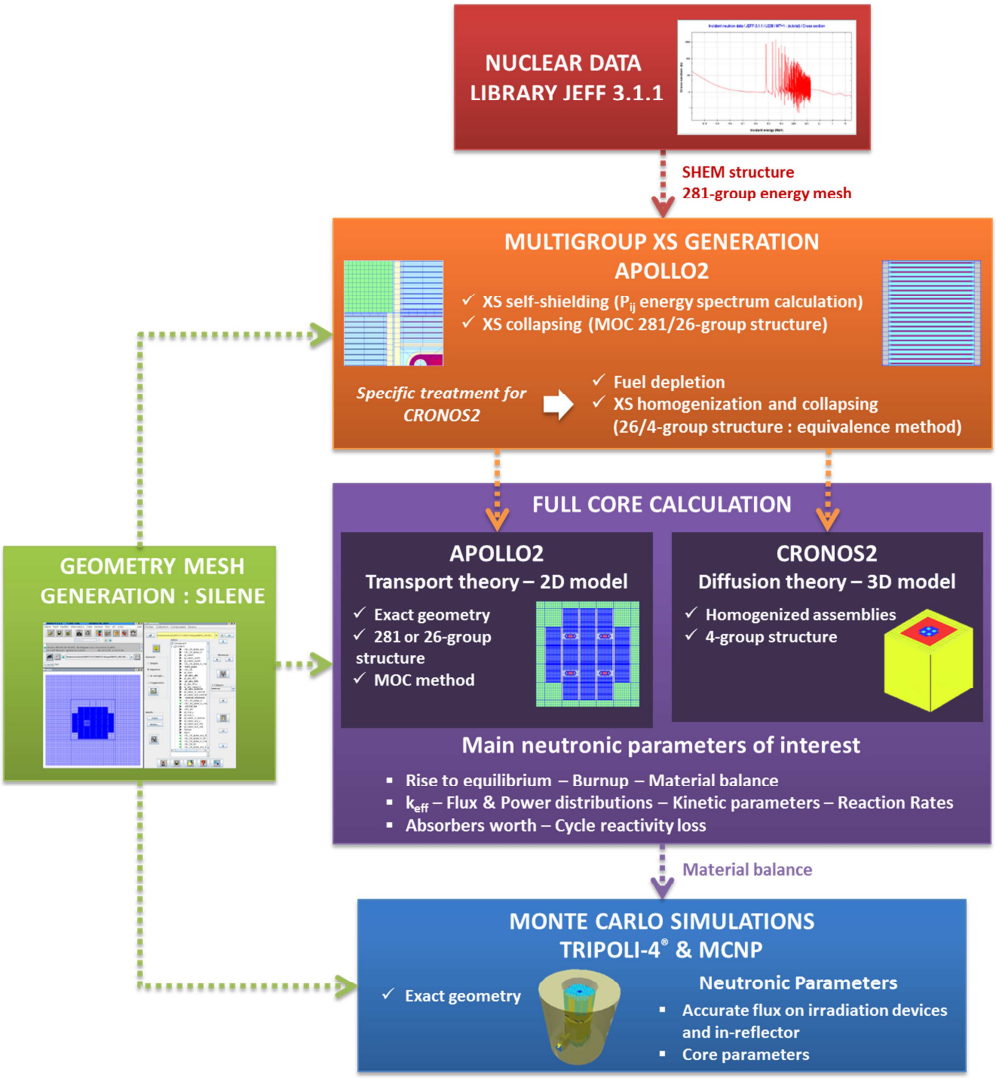

FIG. 2. COCONEUT overview.

3.2 Two Dimensional lattice calculations

With COCONEUT, cross sections are calculated on two types of geometric patterns in two dimensions in infinite lattice. The first geometry is used for computing the Standard Fuel Assembly cross sections (see FIG. 3, left side). The second is used for computing the Absorber Fuel Assembly cross sections. It corresponds to an assembly with control rods withdrawn or inserted surrounded by several SFA (see FIG. 3, right side). The idea is to treat a supercritical configuration with a representative neutronic spectrum diffusing within the AFA.

All results presented in this work have been done using the 26 group cross sections calculation scheme for both the 2D fuel assemblies and core calculations.

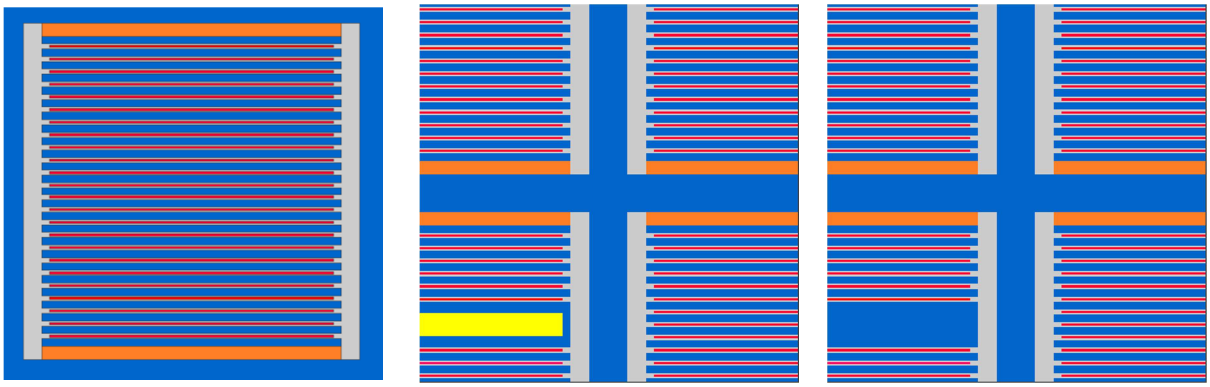

FIG. 3. Fuel assembly lattice configurations: SFA (left), AFA with inserted control rods (middle) and AFA with withdrawn control rods (right).

4. Monte-Carlo Depletion Calculation Code

The idea of Monte Carlo codes is to solve the Boltzmann equation by using only stochastic methods to avoid hypotheses. Every neutron history is tracked and every parameter is sampled. All results are computed by statistical consideration. With the increase of computer performances, it is now possible to perform a fuel depletion calculation, by using Monte Carlo to solve the Boltzmann equation and deterministic tools to solve Bateman equations introducing additional assumptions. TRIPOLI-4®, SERPENT and MCNP Monte Carlo calculation codes are mainly used at TechnicAtome for R&D studies and, in particular, for new Research Reactors design. Each code has its own depletion module, pros and cons.

4.1 General feature

Different methods exist to solve the depletion equation and are well documented in the literature [10]. The predictor-corrector approach is available for the three stochastic codes. It has been chosen for SERPENT and MCNP whereas the Euler method is chosen for TRIPOLI-4® (in order to decrease calculation time). The processes are summarized in FIG. 4. The idea of second order predictor-corrector method is to start with a Monte Carlo calculation at beginning of step (BOS). After a provisional irradiation step (called “predictor”), a neutron transport problem is solved at end of step (EOS), and the average fluxes and cross sections between the BOS and EOS are employed to recalculate the new EOS compositions [11]. The Euler method is simpler: fluxes are calculated at each step and are used to solve Bateman equations to directly compute the next concentration.

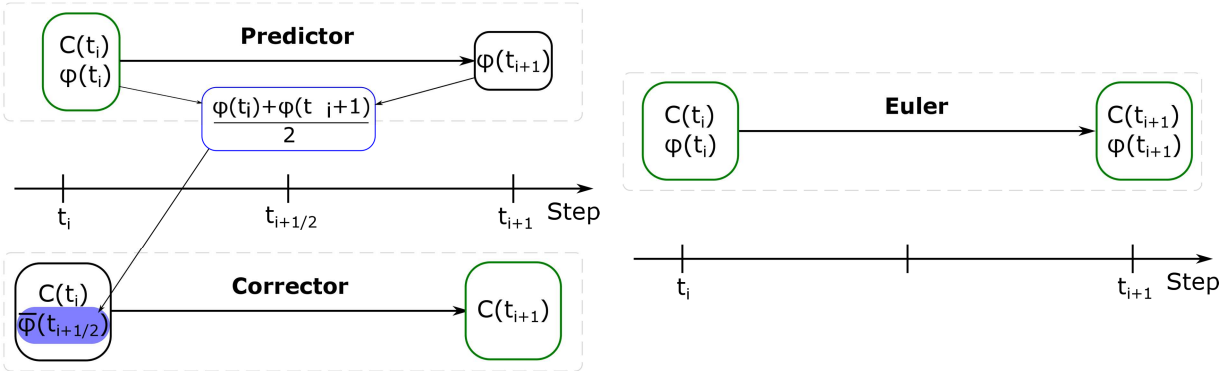

FIG. 4. Predictor-corrector and Euler methods.

For each step, statistical and systematic uncertainties should be taken into account correctly for key parameters (concentration, reactivity worth, fluxes…). However, the systematic uncertainties calculation is not obvious and often asking for high computer performance. Methods exist [12] but are not taken into account in this paper thus uncertainties are not calculated for concentration. Statistical uncertainties for each calculation step do not exceed +/- 40 pcm at 1σ on the reactivity worth.

4.2 TRIPOLI-4®

TRIPOLI-4® depletion capability is made of two C++ interfaces that wrap the functionalities of both TRIPOLI-4® and MENDEL [13]. In addition to these tools consisting in a set of generic methods for MC neutron transport and methods performing material depletion calculation with the fourth order Runge–Kutta method, ROOT scripts allow for dynamically reloading of compositions or even geometry (AFA reshuffling and control rod displacement). All interfaces are linked to the C++ (root C++ interpreter [14]) allowing to build advanced coupling schemes between transport and burnup which are either run interactively or compiled and executed with coupling scripts. ROOT is used to provide and speed up both the visualization and the analysis of the results.

4.3 SERPENT-2

SERPENT-2 [15] is a three-dimensional continuous energy Monte Carlo reactor physics burnup calculation code developed at the VTT Technical Research Centre of Finland since 2004. The code is specialized in lattice physics calculations. The neutron transport is based on a combination of conventional surface-to surface ray-tracing and the Woodcock delta-tracking method [16]. Burnup depletion equations are solved using the matrix exponential method CRAM [17], providing a robust and accurate solution with a very short computation time. A comparison between CRAM, ORIGEN solver and other TTA (Truncated Taylor Approximation) methods proved the advantages of the CRAM method in terms of accuracy and running time, thanks to its mathematical approach [10].

4.4 MCNP-6.1

MCNP code is used worldwide for calculations of multiplication factor, reaction rates, neutron fluxes, power peaking factors, neutronic and gamma heatings. It was commonly used by TechnicAtome during the JHR design [18]. Criticality calculation (using KCODE card) with the “BURN” option card is used in this paper. Depletion is assumed by CINDER-90 [19].

5. Results and analysis

Some key parameters are considered in this study, limiting the high number of physical quantities to analyze. The multiplication coefficient is considered and deduced reactivity worth is calculated using the following formulae:

$$\rho = \left(1 - \frac{1}{k}\right) \cdot 10^5$$

Then reactivity comparison between codes is calculated as follow:

$$\Delta\rho = \rho_1 - \rho_2$$

Results on isotope concentration are provided in overall core or assembly (actinide, fission product and burnable poison). Units are given in 10^{-24} at.cm^{-3}.

5.1 Standard Fuel Assembly

The depletion calculation is done on the standard fuel assembly with three evolving medium for each fuel plate and only one for the boron-aluminum plate. The mesh used has been chosen by looking at the total flux gradient along the plate width. FIG.5 represents this mesh and the total flux.

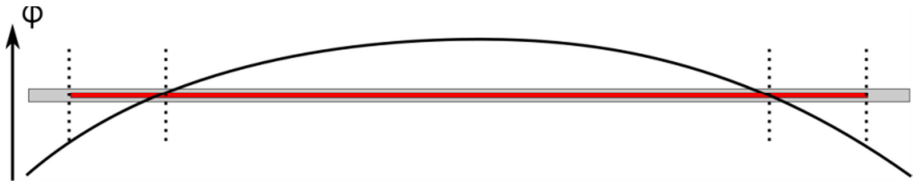

FIG. 5. Mean total flux in a fuel plate and mesh used for the depletion simulation

The k_{inf} evolution of the SFA and reactivity comparison is shown on FIG. 6. All the initial k_{inf} given by the three Monte Carlo codes are all the same within the 1σ range, showing a very good coherent simulation without depletion calculation (see FIG. 6). At the beginning, there is the typical steep gradient on the k_{inf} until fission products concentration reach equilibrium. Concentration of the main anti-reactivity ^{135}Xe (see FIG. 7) is increasing for the first steps and its equilibrium state is reached after 2 days. After this step, ^{10}B burnable poison in the fuel assembly structures is consumed during the irradiation. A maximum reactivity peak at ~64 GWd/tU is reached when less than 10% of ^{10}B concentration remains (see FIG. 7). Total fissile isotope concentration is decreasing with a steady slope because the power is fixed. It is the main reactivity effect at higher burnup, when fission products are at equilibrium and ^{10}B poison is burned. It implies a reactivity steep slope at higher burnup. Those phenomena are well reproduced by the codes. However, discrepancies become visible after 60 GWd/tU, even between stochastic simulations. When looking closer to TRIPOLI-4® reactivity curves, one can see an inflection on the slope. It appears when a larger step is computed (multiplying the length of the burnup step by two). This larger step is not justified when looking at the total flux in FIG. 8. Overall flux gradient versus depletion time is steeper when ^{10}B is consumed and burnup step should not be enlarged. Moreover, such an issue might disappear if a predictor-corrector method was also used for TRIPOLI-4®. Special care should be taken depending on the study case (fuel nature, burnable poison…).

Deterministic results seem to slightly differ from stochastic simulations. For example, the k_{inf} evolution is quite well described at the beginning, with an initial bias of 150 pcm, but after 60 GWd/tU, the curve is straying from stochastics curves (FIG. 6). Maximum reactivity gap is found when ^{10}B is half consumed. Some isotopic concentration comparisons are given in Table I. Because stochastic codes give relatively similar results, it has been chosen to compare COCONEUT to the mean value of the three stochastic codes in the table. The higher the burnup is, the larger discrepancy can been seen within a reasonable range (less than 3%). The deterministic evolution calculation was performed with 26 groups and self-shielding was performed only for the initial step. A new version is under development, taking into account self-shielding along the depletion calculation and based on the SHEM-281 [20] multigroup mesh. A closer look to the six factor formulae and reaction rates might provide some answers and guidance for such geometry with either high moderator ratio or absorber.

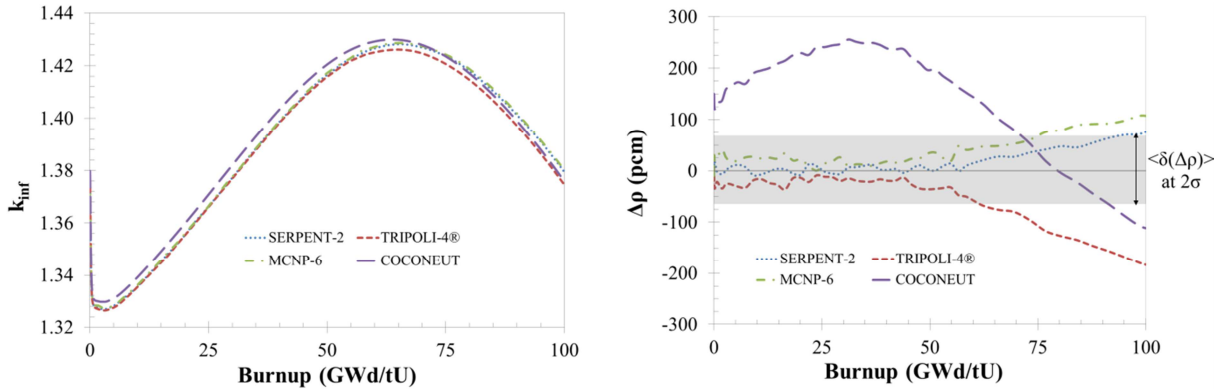

FIG. 6. k_{inf} (left) and reactivity comparison with a mean value of the three Monte Carlo codes as reference (right) in FA. The average stochastic uncertainties on Δρ are represented at 2σ.

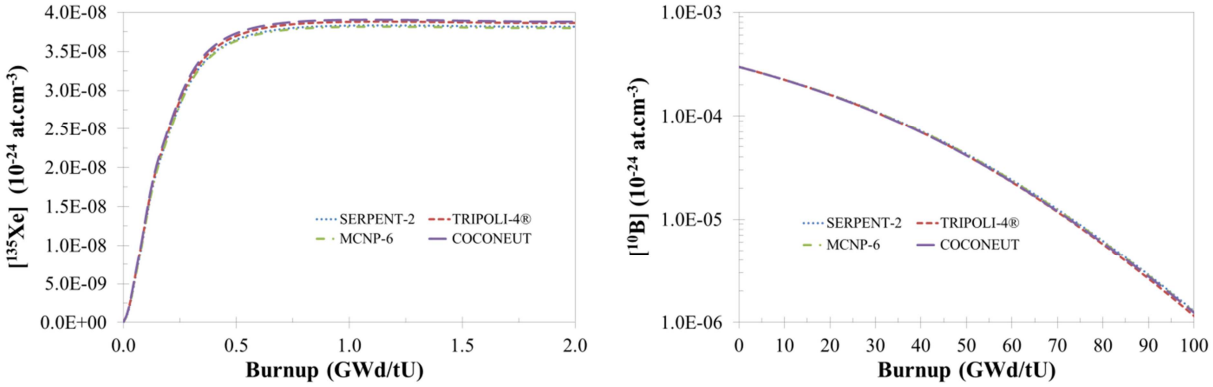

FIG. 7. ^{135}Xe (left) and ^{10}B (right) concentrations in FA.

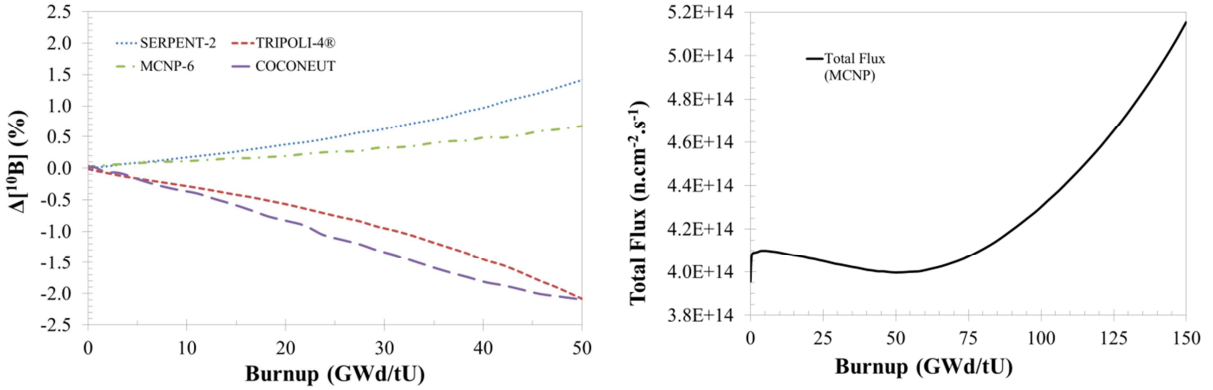

FIG. 8. Relative ^{10}B concentration (left) and MCNP total flux (right) in FA.

TABLE I: Relative concentration comparison (%) between COCONEUT and stochastic codes (mean value of the three simulations) for ^{235}U, ^{239}Pu, ^{148}Nd and ^{149}Sm.

Burnup (GWd/tU)	20	40	60	80	100
$\Delta[^{235}U]$	-0.12	-0.27	-0.46	-0.69	-1.03
$\Delta[^{239}Pu]$	2.42	1.89	1.33	0.82	0.21
$\Delta[^{148}Nd]$	1.95	2.07	2.12	2.14	2.15
$\Delta[^{149}Sm]$	1.36	1.13	1.59	2.03	2.48

5.2 Absorber Fuel Assembly

Same burnup steps as for the SFA have been chosen for those cases. It implies the irradiation time at a given burnup step for the ASA is higher than the one for the SFA because there is less fuel (22.5 fuel plate instead of 24). It implies a slight increase of time step (by ~6%) leading to a higher approximation considered negligible in this study. Similar results have been found for the two AFA cases. Reactivity curves are shifted due to either hafnium absorption (~ -11 300 pcm) or water when they are withdrawn (~ -200 pcm). The high value comes from a 2D consideration, improving considerably the absorber reactivity coefficient. Reactivity comparison curves and k_{inf} for the case with control rods inserted and the one with control rods withdrawn are respectively given in FIG. 9 and FIG. 10. As in the previous section, the three stochastic codes are similar until around 60 GWd/tU where TRIPOLI-4® has an inflection in its curvature. COCONEUT starts with a closer k_{inf} than for the SFA, but has a very similar behavior after. Further studies are required to improve the deterministic scheme, as explained in the previous paragraph.

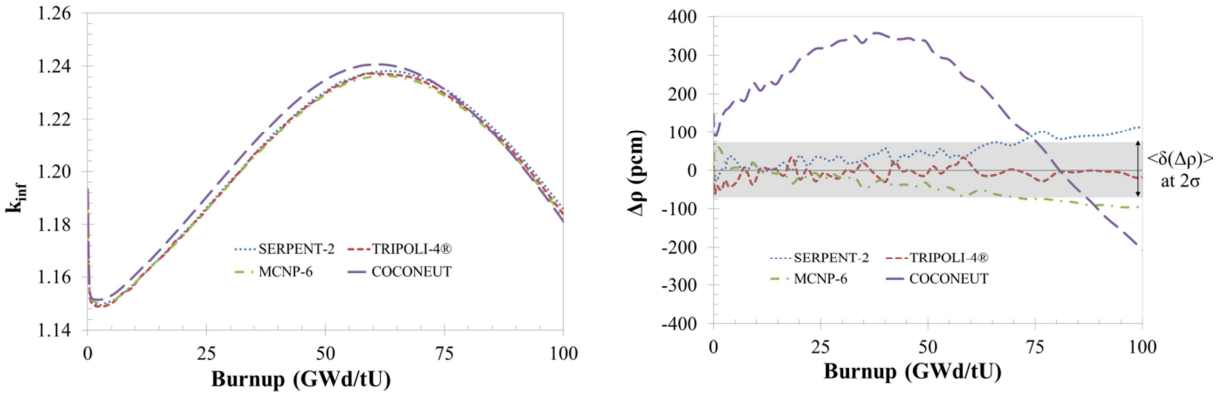

FIG. 9. k_{inf} (left) and reactivity comparison with a mean value of the three Monte Carlo codes as reference (right) in AFA with absorbers inserted.

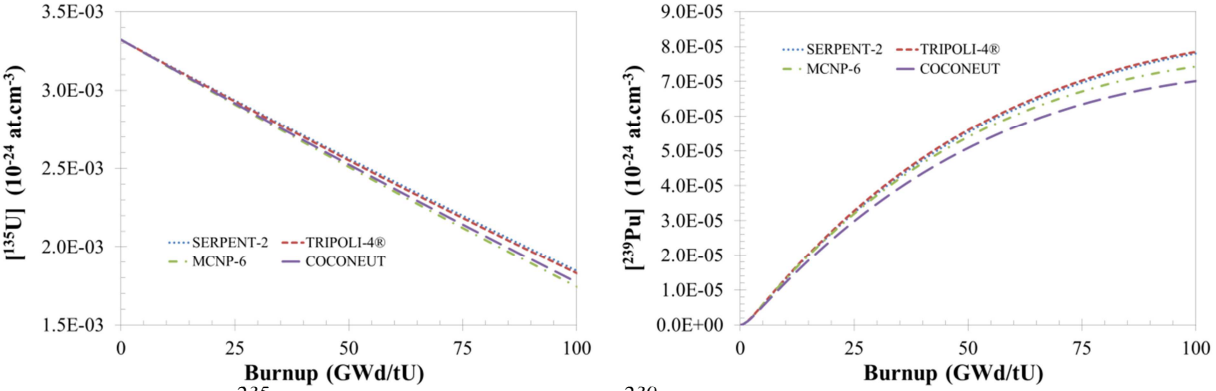

FIG. 10. ^{235}U concentrations (left) and ^{239}Pu concentrations (right) in AFA.

5.4 2D Core calculation

The dummy core has been simulated with only COCONEUT, SERPENT and TRIPOLI-4® codes. One burnable material is considered per fuel plate, leading to 672 depleted medium whereas only 72 and 90 burnable zones were used for respectively the SFA and the AFA. Such simulations require higher storage and calculation time. COCONEUT uses the 26 groups cross sections generated previously by the 2D assembly calculations. Same burnup steps are also used but results are given until 80 GWd/tU.

FIG. 11 shows both the k_{inf} evolution and the reactivity comparisons between COCONEUT, SERPENT and TRIPOLI-4®. All the curves have a very close behavior although a constant bias of -400 pcm is found between deterministic calculation and stochastic simulations. The good agreement can be seen in FIG. 12, where ^{135}Xe and ^{149}Sm reach exactly the same equilibrium between all the codes. Similar observation can be made when looking to the ^{235}U and ^{10}B concentration evolution in FIG. 13.

Those overall good agreements have to be taken carefully. The 2D assembly calculation showed some difference that disappeared in the 2D code calculation. With a constant bias, one can suppose compensation effects are playing a major role. Once again, current deterministic developments with less hypotheses should provide more information on compensations and their origins.

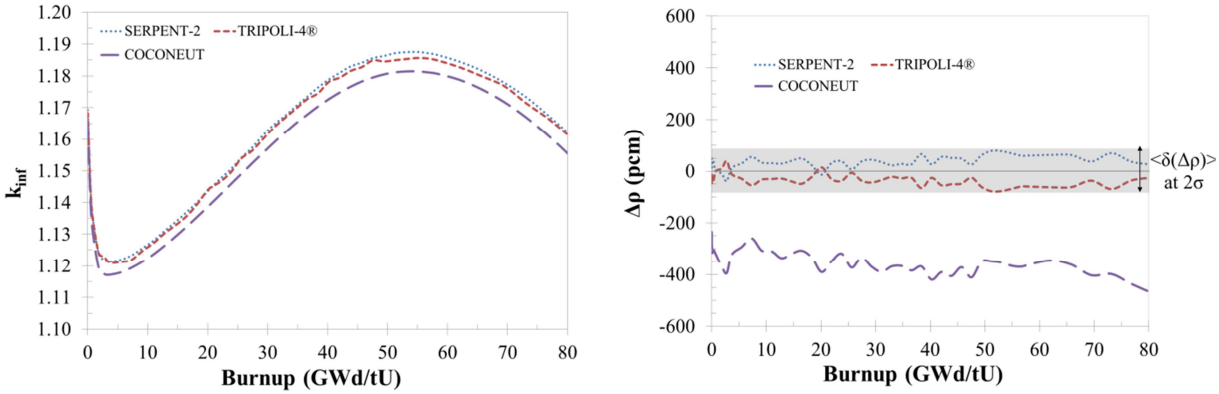

FIG. 11. k_{inf} (left) and reactivity comparison with a mean value of the two Monte Carlo codes as reference (right) for the 2D full core with 16 SFA and 16 AFA with absorbers withdrawn. The average stochastic uncertainties on Δρ (70 pcm) are represented at 2σ.

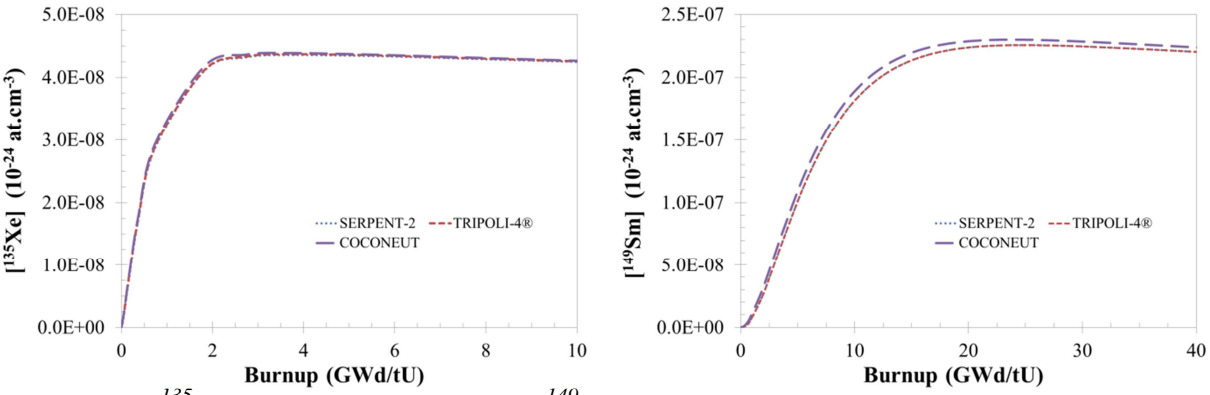

FIG. 12. ^{135}Xe concentration (left) and ^{149}Sm concentrations (right) in the 2D full core.

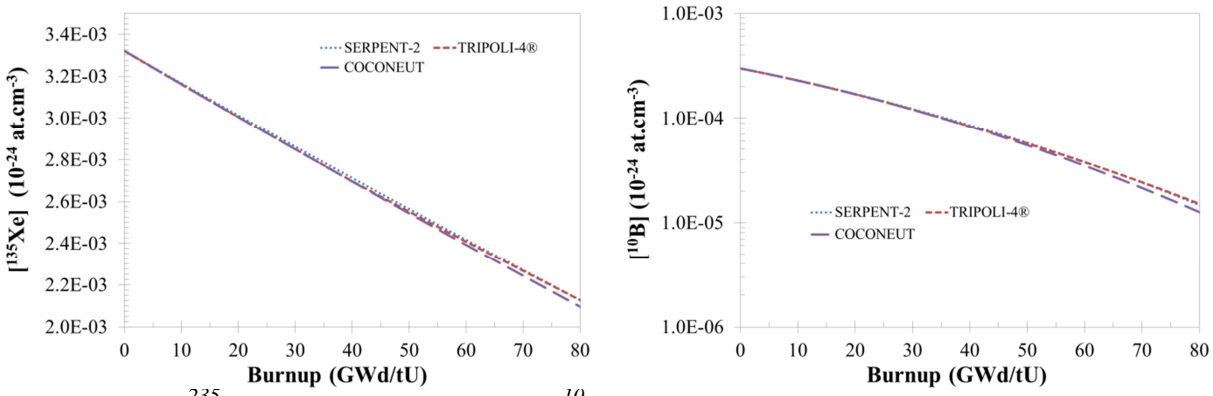

FIG. 13. ^{235}U concentration (left) and ^{10}B concentrations (right) in the 2D full core.

5. Outlooks

Continuous energy Monte Carlo depletion codes still require rather long CPU time in order to carry out very detailed and accurate calculations, even with modern computer technology. To work around this issue, users often have to reduce the number of nuclides in the evolution chains or to consider either longer irradiation time steps and/or larger spatial burn-up cells, limiting the accuracy of the calculation in all cases. The modern SERPENT-2 code allows a time calculation shorter than historical codes, sometimes reducing the length by a factor of 10. It has been shown in this paper the very good agreement between stochastic codes. The second order predictor-corrector method is more accurate than the first order Euler approach: it limits issues on burnup step determination depending on calculation type (fuel, burnable poison…). However, it requires two times more simulations. Some discrepancies have been pointed out on TRIPOLI-4® depletion calculation (using Euler) when there is a change in the step length (doubling the length of the step).

To reduce time calculation for an industrial point of view, TechnicAtome has developed its own deterministic calculation scheme COCONEUT. Results presented along this paper are done in 2D with the pre-conception version. The general behavior compared to stochastic codes is well described. Excellent agreement is observed between COCONEUT and stochastic codes up to 100 GWj/tU.
A new version is under development, taking into account self-shielding along the depletion calculation and based on the SHEM-281 [20] multigroup mesh. Further studies have to be done by looking to the six factor formulae and power maps to guide the developments.

Allowing fuel refueling, changing control rods position (for criticality) and changing depletion mesh step by step for better accuracy considerably enhances the use of Monte Carlo 3D core calculation.

6. Acknowledgements

The authors would like to thanks Carole Seuvre for her help and development around SERPENT code during her internship at TechnicAtome. They are also grateful to the COCONEUT developing team for support and advice.

7. References

[1] Brun, E., et al., "Tripoli-4®, CEA, EDF and AREVA reference Monte Carlo code", Annals of Nuclear Energy, **82** (2013), pp. 151-160.

[2] Goorley, T., et al., "Initial MCNP-6 Release Overview", Nuclear Technology, **180** (2012), pp. 298-315.

[3] Leppänen, J., et al., "The Serpent Monte Carlo code: status, development and applications in 2013", Annals of Nuclear Energy, **82** (2015), pp. 142-150.

[4] Lacombe, J.G, et al., "COCONEUT: Enhancing Neutronic Design for Research Reactor", IGORR-2016 Proceeding, Berlin (2016), *to be published.*

[5] Bouret, C., et al, "COCONEUT: First steps of validation for the new AREVA TA neutronic deterministic scheme for Research Reactor design", IGORR-2016 Proceedings, Berlin (2016), *to be published.*

[6] Sanchez, R., et al. "Apollo2 year 2010", Nuclear Engineering and Technology, **42** (2010), pp. 474-499.

[7] Lautard, J., et al., "CRONOS: a modular computational system for neutronic core calculations", IAEA specialist meeting on advanced calculational methods for power reactors, Cadarache (1990), France.

[8] Nicolas, S., et al., "A dummy core for V&V and education and training purposes at TechnicAtome: in and ex-core calculations", IGORR-2017 Proceedings, Sydney (2017), *to be published.*

[9] Santamarina, A. et al., "The JEFF-3.1.1 Nuclear Data Library", OECD/NEA Data Bank, JEFF Report 22 (2009).

[10] Isolato, A., "Computational Methods for Burnup Calculations with Monte Carlo Neutronics", PhD thesis, Aalto University (2013).

[11] Isolato, A., et al, "Substep methods for burnup calculations with Bateman solutions", Annals of Nuclear Energy, **38** (2011), pp. 2509-2514.

[12] Brun, B., et al., "Systematic Uncertainty Due to Statistics in Monte Carlo Burnup Codes: Application to a Simple Benchmark with TRIPOLI-4-D", Nuclear Science and Technology, **2** (2011), pp. 879-885.

[13] Lahaye, S., et al., "First verification and validation steps of MENDEL Release 1.0 cycle code system", PHYSOR-2014 Proceedings, Kyoto (2014), Korea.

[14] Brun, R., et al., "ROOT - An Object Oriented Data Analysis Framework", Nuclear Instrument and Methods in Physic Research, A**389** (1996), pp. 81-86.

[15] Leppänen, J., et al., "The Serpent Monte Carlo code: Status, development and applications in 2013", Annals of Nuclear Energy, **82** (2015), pp. 142-150.

[16] Leppänen, J., "Performance of Woodcock delta-tracking in lattice physics applications using the Serpent Monte Carlo reactor physics burnup calculation code", Annals of Nuclear Energy, **37** (2010), pp. 715–722.

[17] Pusa, M., et al., "Solving linear systems with sparse Gaussian elimination in the Chebyshev rational approximation method (CRAM)", Nuclear Science and Engineering, **175** (2013), pp. 250-258.

[18] E. Privas et al., "Reflector features and physics consideration of the Jules Horowitz Reactor," Proceeding of the International Topical Meeting on Research Reactor and Fuel Management RRFM 2017, Rotterdam, Netherland, 2017.

[19] W. B. Wilson, et al., "A Manual for CINDER'90 Version 07.4 Codes and Data", LA-UR-07-8412, Los Alamos National Laboratory, USA (2008).

[20] Santamarina, A., et al., "The SHEM energy mesh for accurate fuel depletion and BUC calculations", International Conference on Nuclear Criticality-Safety, St Petersburg (2007), Russia.