Validation of APOLLO2 toward Monte Carlo TRIPOLI-4 throughout irradiation: transposition of the process on critical fuel assembly configurations
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VALIDATION OF APOLLO2 TOWARD MONTE CARLO TRIPOLI-4® THROUGHOUT IRRADIATION: TRANSPOSITION OF THE PROCESS ON CRITICAL FUEL ASSEMBLY CONFIGURATIONS

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Context:

- Current usual PWR neutronic simulations rely on two-step calculation schemes:
  - 2D lattice calculation on an infinitely repeated pattern (e.g. an assembly),
  - 3D core calculation with homogenized cross sections given by the first step.

- The numerical validation process is based on comparisons with reference calculations (Monte Carlo) at different geometrical scales.

- Comparisons at the assembly level between deterministic and reference models are usually performed considering a zero-buckling assumption.

- Validity of the transposition of the validation process results to critical-buckling configurations?
INTRODUCTION: IMPACT OF THE CRITICAL-BUCKLING ASSUMPTION

- Comparisons at the assembly level between deterministic and reference models are usually performed considering a zero-buckling assumption.

- The impact of the leakage model can be significant.

In APOLLO2, zero-buckling vs critical-buckling (homogeneous B1):

- Shift in the energy neutron spectrum up to a few percent between thermal and fast components.

- It follows discrepancies in terms of reactivity, fission rate distribution, neutron delayed fraction and isotopic balance.

- In this work, we will investigate the impact of the leakage model by solving an albedo-eigenvalue problem.
1. Description of the modelling tools
   a) Deterministic calculations in APOLLO2
   b) Monte Carlo calculations in TRIPOLI-4®
   c) Leakage model for lattice configurations

2. Analysis of the results for static configurations

3. Analysis of the results throughout irradiation

4. Conclusion and perspective
• In this work, typical 17x17 pins assemblies are considered with various fuel enrichments (from 3.25 to 4.95 wt.% U\textsuperscript{235}/U).

• The main features of the deterministic calculation scheme in APOLLO2 are as follows:
  - JEFF3.1.1 cross section library.
  - Method of Characteristics (MOC) solver.
  - 281 energy groups (SHEM).

• Depletion geometry: 4 rings in fuel pins.
MONTE CARLO CALCULATIONS IN TRIPOLI-4®

- Monte Carlo simulations are performed with TRIPOLI-4® coupled with MENDEL for depletion calculation (same depletion geometry as in APOLLO2 is used).
- Uncertainty propagation is carried out by running independent simulations:

SIMULATION 1

- Data preparation for irradiation step (i)
  - Modification of the depleting media composition

Monte-Carlo Transport Calculation
TRIPOLI-4
N particles simulated – Calculation of the reaction rates of flux calculation for the selected isotopes

Depletion Calculation
(Fissile & burnable poison)
MENDEL

SIMULATION M

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MENDEL

Iteration over time steps
THE ALBEDO LEAKAGE MODEL

- B1 leakage model’s implementation non trivial in Monte Carlo when ensuring the consistency with respect to deterministic solvers.
- Whereas the albedo leakage method can be implemented without any code specific approximations.
- In such a method, the $k_{\text{eff}}$-eigenvalue problem is changed to a $(1-\alpha)$-eigenvalue problem, where $\alpha$ is the albedo defined as:

$$\alpha = \frac{\phi(\vec{r}, \vec{\Omega}', E')}{\phi(\vec{r}, \vec{\Omega}, E')}$$

for $\vec{n}.\vec{\Omega}' = -\vec{n}.\vec{\Omega} < 0, \vec{r} \in \Gamma$ ($\Gamma$ being the boundary of the system)

- The problem is solved iteratively until the convergence to the criticality is reached:

$$\alpha_{n+1} = \frac{k}{\alpha_n^a}, \quad \text{with } a = \frac{1}{2}$$
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3. Analysis of the results throughout irradiation

4. Conclusion and perspective
• Impact of the leakage adjustment on the fission rate distribution for fresh fuel enriched at 3.25 wt.% U$^{235}$/U (in APOLLO2).

  ➢ Shift towards the assembly center.

• Because of the shift of the energy spectrum, the average neutron delayed fraction increases by 7% to 8% (see next slides).
• Small reactivity discrepancies (<150 pcm).
• Good agreement of the neutron energy spectra and fission rate distributions.

Comparaisons between deterministic and Monte Carlo fresh fuel calculation results under zero Buckling assumption at different enrichments

<table>
<thead>
<tr>
<th>Enrichment</th>
<th>Tripoli-4® k_{\text{infinity}}</th>
<th>k_{\text{effective}}</th>
<th>β_{\text{effective}}</th>
<th>Fiss/Capt</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.25 wt.%</td>
<td>1.26674</td>
<td>1.26674</td>
<td>706</td>
<td>1.05923</td>
</tr>
<tr>
<td>4 wt.%</td>
<td>1.31507</td>
<td>1.31507</td>
<td>706</td>
<td>1.14664</td>
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<tr>
<td>4.95 wt.%</td>
<td>1.35941</td>
<td>1.35941</td>
<td>700</td>
<td>1.23361</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Enrichment</th>
<th>Apollo2 k_{\text{infinity}}</th>
<th>k_{\text{effective}}</th>
<th>Δρ (pcm)</th>
<th>Rel Discr (%)</th>
<th>Rel Discr (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.25 wt.%</td>
<td>1.26526</td>
<td>1.26529</td>
<td>92</td>
<td>0.39</td>
<td>0.21</td>
</tr>
<tr>
<td>4 wt.%</td>
<td>1.31354</td>
<td>1.31357</td>
<td>89</td>
<td>0.60</td>
<td>0.22</td>
</tr>
<tr>
<td>4.95 wt.%</td>
<td>1.35689</td>
<td>1.35691</td>
<td>137</td>
<td>0.11</td>
<td>0.40</td>
</tr>
</tbody>
</table>
• Small reactivity discrepancies (<150 pcm): no drift observed!

• Good agreement of the neutron energy spectra and delayed fraction.

• Significant discrepancies in the fission rates in the corner (reduced to 1.4 % by using P3 approximation).

### Comparaisons between deterministic and Monte Carlo fresh fuel calculation results with critical albedo search at different enrichments

<table>
<thead>
<tr>
<th>Tripoli-4®</th>
<th>$k_{\infty}$</th>
<th>$k_{\text{effective}}$</th>
<th>$\beta_{\text{effective}}$</th>
<th>Fiss/Capt</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.25 wt.%</td>
<td>1.25391</td>
<td>1.00011</td>
<td>751</td>
<td>1.03</td>
</tr>
<tr>
<td>4 wt.%</td>
<td>1.30071</td>
<td>1.00010</td>
<td>761</td>
<td>1.11</td>
</tr>
<tr>
<td>4.95 wt.%</td>
<td>1.34477</td>
<td>1.00009</td>
<td>755</td>
<td>1.20</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Apollo2</th>
<th>$k_{\infty}$</th>
<th>$k_{\text{effective}}$</th>
<th>$\Delta \rho$ (pcm)</th>
<th>Rel Discr (%)</th>
<th>Rel Discr (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.25 wt.%</td>
<td>1.25242</td>
<td>0.99994</td>
<td>95</td>
<td>0.66</td>
<td>0.21</td>
</tr>
<tr>
<td>4 wt.%</td>
<td>1.29958</td>
<td>1.00005</td>
<td>67</td>
<td>1.07</td>
<td>0.16</td>
</tr>
<tr>
<td>4.95 wt.%</td>
<td>1.34259</td>
<td>0.99991</td>
<td>121</td>
<td>0.68</td>
<td>0.33</td>
</tr>
</tbody>
</table>

### Relative discrepancies on the neutron energy spectrum for fresh fuel with critical albedo search (APOLLO2 vs TRIPOLI-4®)

### Relative discrepancies of fission rates for fresh fuel with critical albedo search (APOLLO2 vs TRIPOLI-4®)
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3. Analysis of the results throughout irradiation

4. Conclusion and perspective
• Impact of the leakage adjustment on the reactivity along depletion in APOLLO2 (fuel enriched at 3.25 wt.% $^{235}\text{U}/\text{U}$).
  ➢ Significant impact on the reactivity: from -900 pcm to +500 pcm.

• It also impacts the concentrations of main heavy isotopes (up to 2% for $^{239}\text{Pu}$).
• Good agreement between deterministic and Monte Carlo results [-140 pcm; -60 pcm].

• No significant drift during irradiation.

• The same conclusion is drawn concerning the average delayed neutron fraction: it falls within the ±3σ of the Monte Carlo computation.

• Various U235 enrichments have been tested and lead to the same observations.

• Confirms the consistency of deterministic simulations regardless of the leakage model.

Reactivity discrepancies during irradiation (APOLLO2 vs TRIPOLI-4®)
- Discrepancies in isotopic compositions amount to the percent level for Pu$^{240}$ and Pu$^{241}$.
- Same order of magnitude for both methods (with or without critical leakage).
- Confirms as well the consistency of deterministic simulations regardless of the leakage model.
Achievements

- A consistent critical leakage method has been implemented both in Monte Carlo and in deterministic codes, namely the critical albedo adjustment.
- The analysis was performed for various fuel enrichments and irradiated compositions.
- The discrepancies on main neutronic parameters do not rise in critical leakage configurations.

Perspective

- Test the method on different assembly types including MOX fuel and burnable poisons.
Thank you for your attention