Validation of APOLLO2 toward Monte Carlo TRIPOLI-4 throughout irradiation: transposition of the process on critical fuel assembly configurations

F. Damian, A. Collin, N. Gerard-Castaing, C. Jouglard, A. Zoia

DE LA RECHERCHE À L'INDUSTRIE

VALIDATION OF APOLLO2 TOWARD MONTE CARLO TRIPOLI-4® THROUGHOUT IRRADIATION :

TRANSPOSITION OF THE PROCESS ON CRITICAL FUEL ASSEMBLY CONFIGURATIONS

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INTRODUCTION: PROBLEM CONTEXT

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?

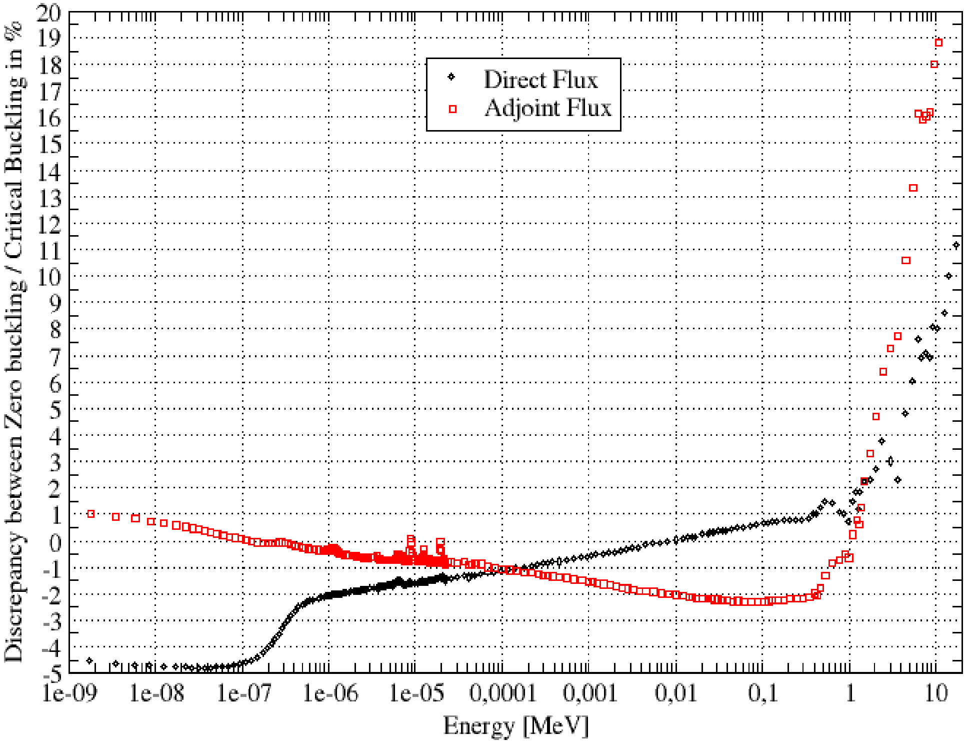
INTRODUCTION: IMPACT OF THE CRITICAL-BUCKLING ASSUMPTION

- 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.

OUTLINE

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

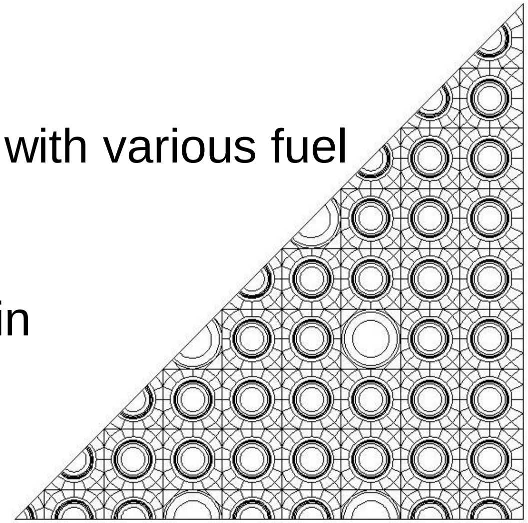
4. Conclusion and perspective

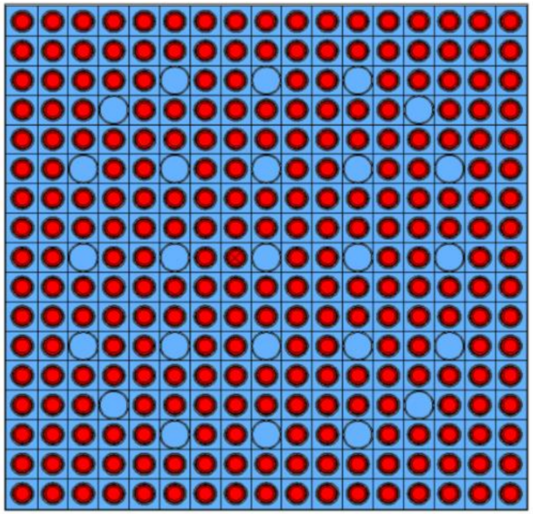
DETERMINISTIC CALCULATIONS IN APOLLO2

- In this work, typical 17x17 pins assemblies are considered with various fuel enrichments (from 3.25 to 4.95 wt.% U^{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).

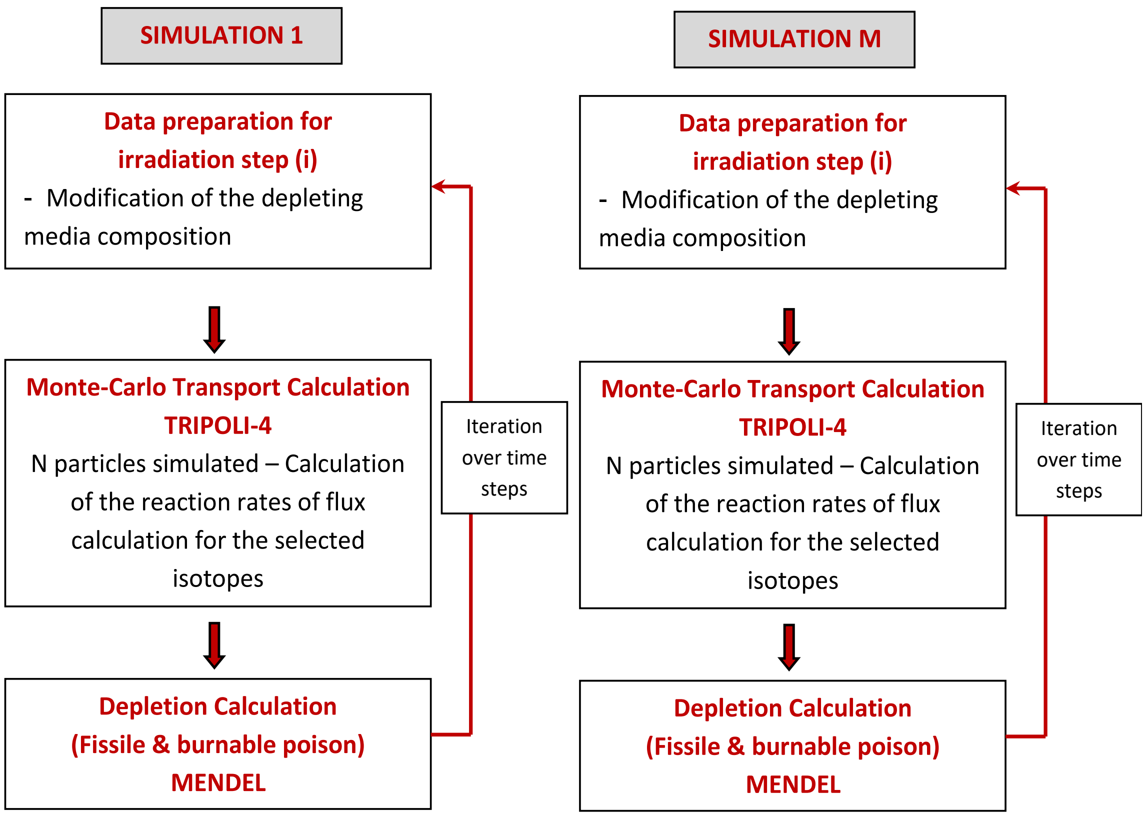
- Depletion geometry: 4 rings in fuel pins.





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:



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_{eff}-eigenvalue problem is changed to a (1-α)-eigen-value problem, where α is the albedo defined as:

$$\alpha = \frac{\phi\left(\vec{r}, \overrightarrow{\Omega'}, E'\right)}{\phi\left(\vec{r}, \vec{\Omega}, E'\right)}, for\ \vec{n}.\overrightarrow{\Omega'} = -\vec{n}.\vec{\Omega} < 0, \vec{r} \in \Gamma\ (\Gamma \text{ being the boundray of the system})$$

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

$$\alpha_{n+1} = \frac{k}{\alpha_n^a}, \qquad with\ a = \frac{1}{2}$$

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IMPACT OF THE CRITICAL ALBEDO SEARCH: STATIC CALCULATIONS

- 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.

0,95	0,94	0,95	0,96	0,97	0,98	0,98	0,98	0,98	0,98	0,98	0,98	0,97	0,96	0,95	0,94	0,95
0,94	0,94	0,95	0,97	0,99	1,02	0,99	0,99	1,02	0,99	0,99	1,02	0,99	0,97	0,95	0,94	0,94
0,95	0,95	0,98	1,02	1,04		1,03	1,03		1,03	1,03		1,04	1,02	0,98	0,95	0,95
0,96	0,97	1,02		1,06	1,05	1,01	1,01	1,04	1,01	1,01	1,05	1,06		1,02	0,97	0,96
0,97	0,99	1,04	1,06	1,04	1,05	1,02	1,01	1,04	1,01	1,02	1,05	1,04	1,06	1,04	0,99	0,97
0,98	1,02		1,05	1,05		1,04	1,04		1,04	1,04		1,05	1,05		1,02	0,98
0,98	0,99	1,03	1,01	1,02	1,04	1,02	1,01	1,04	1,01	1,02	1,04	1,02	1,01	1,03	0,99	0,98
0,98	0,99	1,03	1,01	1,01	1,04	1,01	1,01	1,04	1,01	1,01	1,04	1,01	1,01	1,03	0,99	0,98
0,98	1,02		1,04	1,04		1,04	1,04		1,04	1,04		1,04	1,04		1,02	0,98
0,98	0,99	1,03	1,01	1,01	1,04	1,01	1,01	1,04	1,01	1,01	1,04	1,01	1,01	1,03	0,99	0,98
0,98	0,99	1,03	1,01	1,02	1,04	1,02	1,01	1,04	1,01	1,02	1,04	1,02	1,01	1,03	0,99	0,98
0,98	1,02		1,05	1,05		1,04	1,04		1,04	1,04		1,05	1,05		1,02	0,98
0,97	0,99	1,04	1,06	1,04	1,05	1,02	1,01	1,04	1,01	1,02	1,05	1,04	1,06	1,04	0,99	0,97
0,96	0,97	1,02		1,06	1,05	1,01	1,01	1,04	1,01	1,01	1,05	1,06		1,02	0,97	0,96
0,95	0,95	0,98	1,02	1,04		1,03	1,03		1,03	1,03		1,04	1,02	0,98	0,95	0,95
0,94	0,94	0,95	0,97	0,99	1,02	0,99	0,99	1,02	0,99	0,99	1,02	0,99	0,97	0,95	0,94	0,94
0,95	0,94	0,95	0,96	0,97	0,98	0,98	0,98	0,98	0,98	0,98	0,98	0,97	0,96	0,95	0,94	0,95

0,70	0,75	0,80	0,83	0,86	0,89	0,90	0,91	0,91	0,91	0,90	0,89	0,86	0,83	0,80	0,75	0,70
0,75	0,81	0,86	0,90	0,95	0,99	0,98	0,99	1,01	0,99	0,98	0,99	0,95	0,90	0,86	0,81	0,75
0,80	0,86	0,92	1,00	1,04		1,06	1,07		1,07	1,06		1,04	1,00	0,92	0,86	0,80
0,83	0,90	1,00		1,09	1,10	1,08	1,08	1,11	1,08	1,08	1,10	1,09		1,00	0,90	0,83
0,86	0,95	1,04	1,09	1,10	1,13	1,11	1,11	1,14	1,11	1,11	1,13	1,10	1,09	1,04	0,95	0,86
0,89	0,99		1,10	1,13		1,16	1,16		1,16	1,16		1,13	1,10		0,99	0,89
0,90	0,98	1,06	1,08	1,11	1,16	1,14	1,15	1,18	1,15	1,14	1,16	1,11	1,08	1,06	0,98	0,90
0,91	0,99	1,07	1,08	1,11	1,16	1,15	1,15	1,19	1,15	1,15	1,16	1,11	1,08	1,07	0,99	0,91
0,91	1,01		1,11	1,14		1,18	1,19		1,19	1,18		1,14	1,11		1,01	0,91
0,91	0,99	1,07	1,08	1,11	1,16	1,15	1,15	1,19	1,15	1,15	1,16	1,11	1,08	1,07	0,99	0,91
0,90	0,98	1,06	1,08	1,11	1,16	1,14	1,15	1,18	1,15	1,14	1,16	1,11	1,08	1,06	0,98	0,90
0,89	0,99		1,10	1,13		1,16	1,16		1,16	1,16		1,13	1,10		0,99	0,89
0,86	0,95	1,04	1,09	1,10	1,13	1,11	1,11	1,14	1,11	1,11	1,13	1,10	1,09	1,04	0,95	0,86
0,83	0,90	1,00		1,09	1,10	1,08	1,08	1,11	1,08	1,08	1,10	1,09		1,00	0,90	0,83
0,80	0,86	0,92	1,00	1,04		1,06	1,07		1,07	1,06		1,04	1,00	0,92	0,86	0,80
0,75	0,81	0,86	0,90	0,95	0,99	0,98	0,99	1,01	0,99	0,98	0,99	0,95	0,90	0,86	0,81	0,75
0,70	0,75	0,80	0,83	0,86	0,89	0,90	0,91	0,91	0,91	0,90	0,89	0,86	0,83	0,80	0,75	0,70

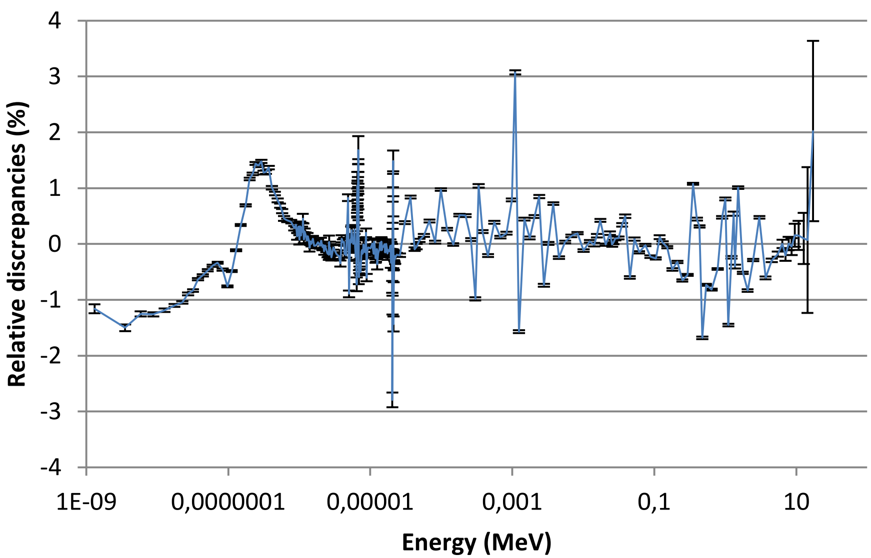
- Because of the shift of the energy spectrum, the average neutron delayed fraction increases by 7% to 8% (see next slides).

STATIC CALCULATIONS – ZERO BUCKLING ASSUMPTION

- Small reactivity discrepancies (<150 pcm).
- Good agreement of the neutron energy spectra and fission rate distributions.

Tripoli-4®	$k_{infinity}$	$k_{effective}$		$\beta_{effective}$	Fiss/Capt
3.25 wt.%	1.26674	1.26674		706	1.05923
4 wt.%	1.31507	1.31507		706	1.14664
4.95 wt.%	1.35941	1.35941		700	1.23361
Apollo2	$k_{infinity}$	$k_{effective}$	$\Delta\rho$ (pcm)	Rel Discr (%)	Rel Discr (%)
3.25 wt.%	1.26526	1.26529	92	0.39	0.21
4 wt.%	1.31354	1.31357	89	0.60	0.22
4.95 wt.%	1.35689	1.35691	137	0.11	0.40

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



Relative discrepancies on the neutron energy spectrum for fresh fuel under zero buckling assumption (APOLLO2 vs TRIPOLI-4®)

0,10	0,09	0,18	0,02	0,17	0,11	0,04	0,06	0,10	0,06	0,04	0,11	0,17	0,02	0,18	0,09	0,10
0,09	0,32	0,01	0,18	0,15	0,02	0,13	0,06	0,07	0,06	0,13	0,02	0,15	0,18	0,01	0,32	0,09
0,18	0,01	0,15	0,05	0,02		0,01	0,01		0,01	0,01		0,02	0,05	0,15	0,01	0,18
0,02	0,18	0,05		0,03	0,12	0,01	0,01	0,02	0,01	0,01	0,12	0,03		0,05	0,18	0,02
0,17	0,15	0,02	0,03	0,09	0,01	0,00	0,02	0,15	0,02	0,00	0,01	0,09	0,03	0,02	0,15	0,17
0,11	0,02		0,12	0,01		0,10	0,16		0,16	0,10		0,01	0,12		0,02	0,11
0,04	0,13	0,01	0,01	0,00	0,10	0,17	0,03	0,19	0,03	0,17	0,10	0,00	0,01	0,01	0,13	0,04
0,06	0,06	0,01	0,01	0,02	0,16	0,03	0,10	0,17	0,10	0,03	0,16	0,02	0,01	0,01	0,06	0,06
0,10	0,07		0,02	0,15		0,19	0,17		0,17	0,19		0,15	0,02		0,07	0,10
0,06	0,06	0,01	0,01	0,02	0,16	0,03	0,10	0,17	0,10	0,03	0,16	0,02	0,01	0,01	0,06	0,06
0,04	0,13	0,01	0,01	0,00	0,10	0,17	0,03	0,19	0,03	0,17	0,10	0,00	0,01	0,01	0,13	0,04
0,11	0,02		0,12	0,01		0,10	0,16		0,16	0,10		0,01	0,12		0,02	0,11
0,17	0,15	0,02	0,03	0,09	0,01	0,00	0,02	0,15	0,02	0,00	0,01	0,09	0,03	0,02	0,15	0,17
0,02	0,18	0,05		0,03	0,12	0,01	0,01	0,02	0,01	0,01	0,12	0,03		0,05	0,18	0,02
0,18	0,01	0,15	0,05	0,02		0,01	0,01		0,01	0,01		0,02	0,05	0,15	0,01	0,18
0,09	0,32	0,01	0,18	0,15	0,02	0,13	0,06	0,07	0,06	0,13	0,02	0,15	0,18	0,01	0,32	0,09
0,10	0,09	0,18	0,02	0,17	0,11	0,04	0,06	0,10	0,06	0,04	0,11	0,17	0,02	0,18	0,09	0,10

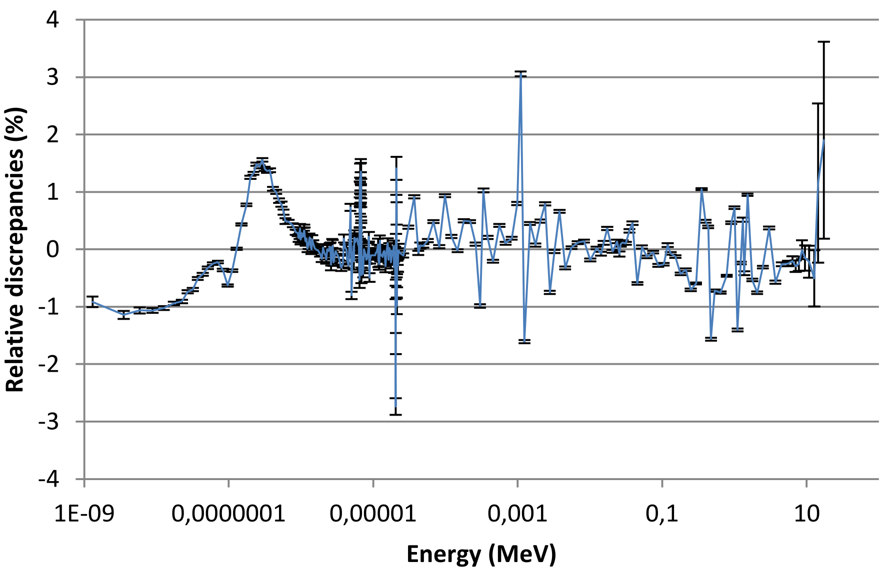
Relative discrepancies of fission rates for fresh fuel under zero Buckling assumption (APOLLO2 vs TRIPOLI-4®)

STATIC CALCULATIONS – CRITICAL ALBEDO SEARCH

- 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).

Tripoli-4®	$k_{infinity}$	$k_{effective}$		$\beta_{effective}$	Fiss/Capt
3.25 wt.%	1.25391	1.00011		751	1.03
4 wt.%	1.30071	1.00010		761	1.11
4.95 wt.%	1.34477	1.00009		755	1.20
Apollo2	**$k_{infinity}$**	**$k_{effective}$**	**Δρ (pcm)**	**Rel Discr (%)**	**Rel Discr (%)**
3.25 wt.%	1.25242	0.99994	95	0.66	0.21
4 wt.%	1.29958	1.00005	67	1.07	0.16
4.95 wt.%	1.34259	0.99991	121	0.68	0.33

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



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

2,45	1,24	0,70	0,22	0,10	0,13	0,19	0,21	0,22	0,21	0,19	0,13	0,10	0,22	0,70	1,24	2,45
1,24	0,87	0,44	0,24	0,01	0,05	0,09	0,21	0,10	0,21	0,09	0,05	0,01	0,24	0,44	0,87	1,24
0,70	0,44	0,29	0,19	0,08		0,05	0,13		0,13	0,05		0,08	0,19	0,29	0,44	0,70
0,22	0,24	0,19		0,15	0,04	0,32	0,23	0,14	0,23	0,32	0,04	0,15		0,19	0,24	0,22
0,10	0,01	0,08	0,15	0,40	0,11	0,09	0,26	0,06	0,26	0,09	0,11	0,40	0,15	0,08	0,01	0,10
0,13	0,05		0,04	0,11		0,14	0,14		0,14	0,14		0,11	0,04		0,05	0,13
0,19	0,09	0,05	0,32	0,09	0,14	0,21	0,30	0,16	0,30	0,21	0,14	0,09	0,32	0,05	0,09	0,19
0,21	0,21	0,13	0,23	0,26	0,14	0,30	0,27	0,02	0,27	0,30	0,14	0,26	0,23	0,13	0,21	0,21
0,22	0,10		0,14	0,06		0,16	0,02		0,02	0,16		0,06	0,14		0,10	0,22
0,21	0,21	0,13	0,23	0,26	0,14	0,30	0,27	0,02	0,27	0,30	0,14	0,26	0,23	0,13	0,21	0,21
0,19	0,09	0,05	0,32	0,09	0,14	0,21	0,30	0,16	0,30	0,21	0,14	0,09	0,32	0,05	0,09	0,19
0,13	0,05		0,04	0,11		0,14	0,14		0,14	0,14		0,11	0,04		0,05	0,13
0,10	0,01	0,08	0,15	0,40	0,11	0,09	0,26	0,06	0,26	0,09	0,11	0,40	0,15	0,08	0,01	0,10
0,22	0,24	0,19		0,15	0,04	0,32	0,23	0,14	0,23	0,32	0,04	0,15		0,19	0,24	0,22
0,70	0,44	0,29	0,19	0,08		0,05	0,13		0,13	0,05		0,08	0,19	0,29	0,44	0,70
1,24	0,87	0,44	0,24	0,01	0,05	0,09	0,21	0,10	0,21	0,09	0,05	0,01	0,24	0,44	0,87	1,24
2,45	1,24	0,70	0,22	0,10	0,13	0,19	0,21	0,22	0,21	0,19	0,13	0,10	0,22	0,70	1,24	2,45

Relative discrepancies of fission rates for fresh fuel with critical albedo search (APOLLO2 vs TRIPOLI-4®)

OUTLINE

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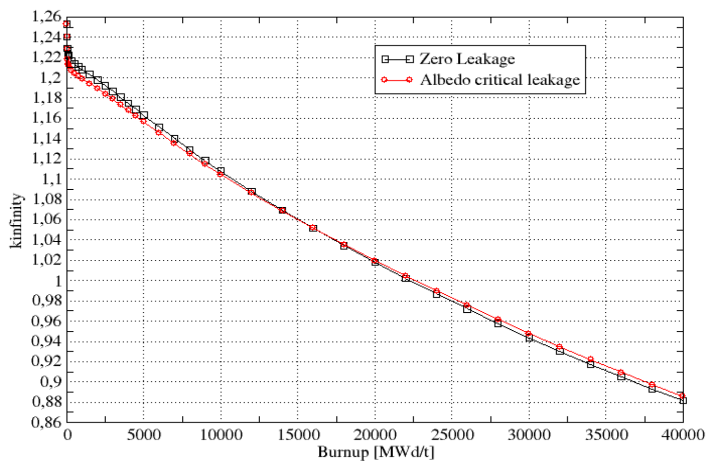
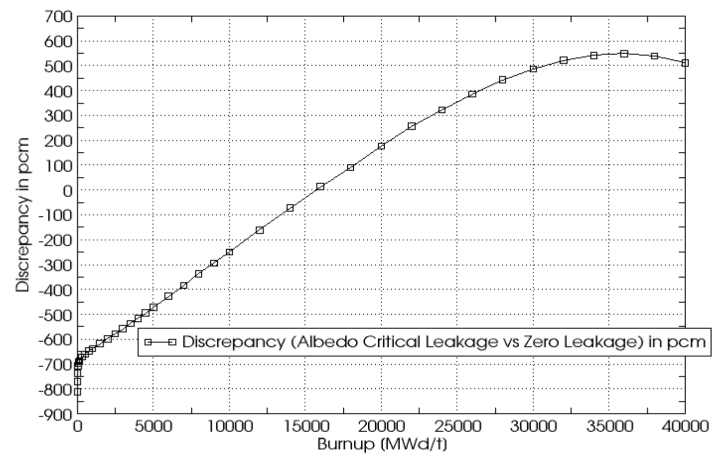
3. **Analysis of the results throughout irradiation**
4. Conclusion and perspective

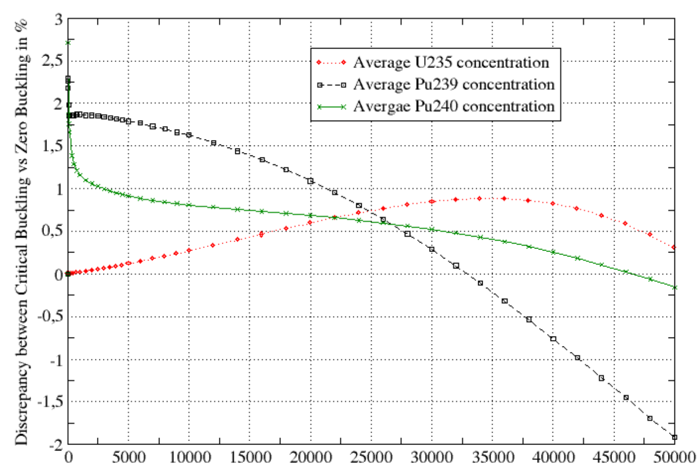
IMPACT OF THE CRITICAL ALBEDO SEARCH: DEPLETION CALCULATIONS

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



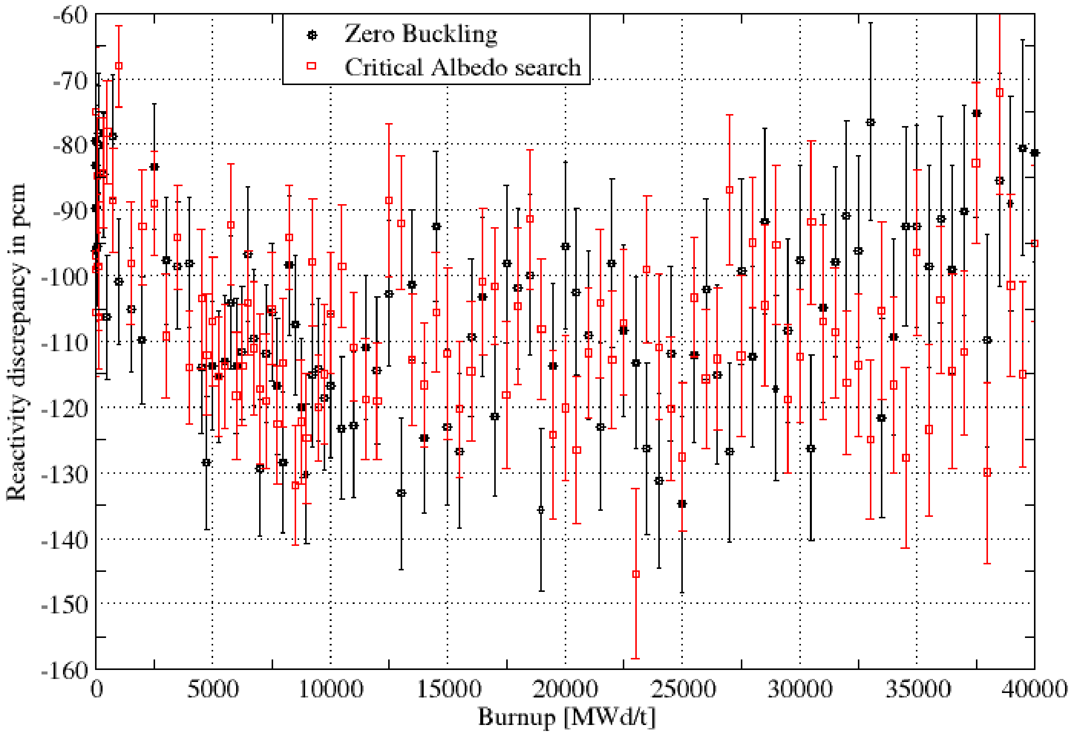


- It also impacts the concentrations of main heavy isotopes (up to 2% for Pu^{239}).



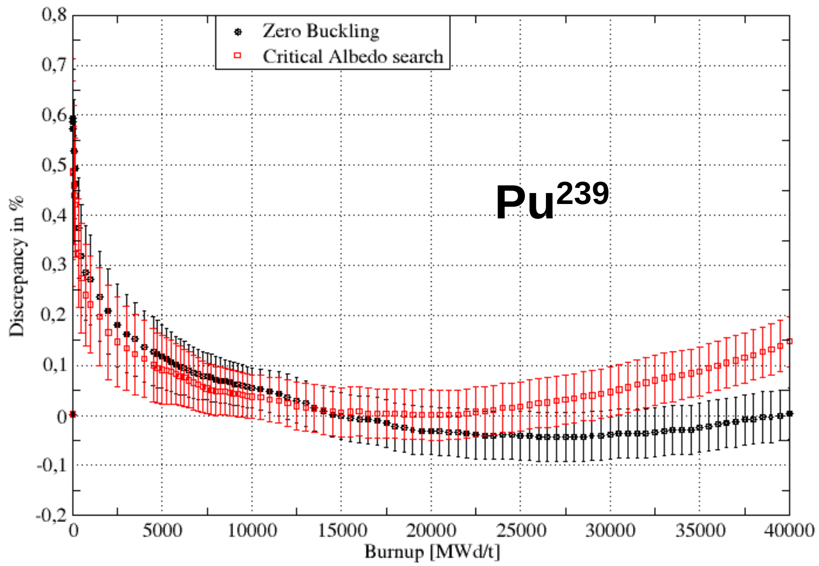
DEPLETION CALCULATIONS

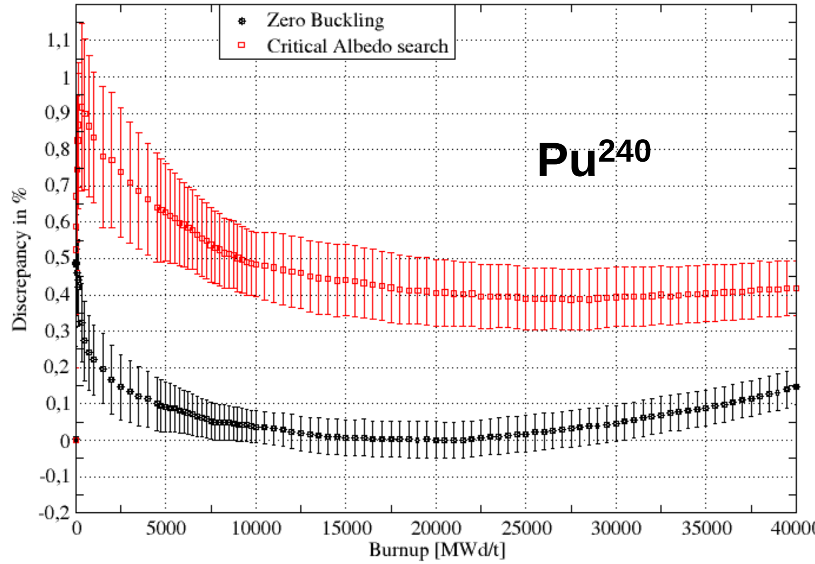
- Good agreement between deterministic and Monte Carlo results [-140 pcm; -60 pcm].
- No significant drift during irradiation.
- The same conclusion is drawn concerning the average delayed neutron fraction: it falls within the ±3σ of the Monte Carlo computation.
- Various U235 enrichments have been tested and lead to the same observations.
- Confirms the consistency of deterministic simulations regardless of the leakage model.



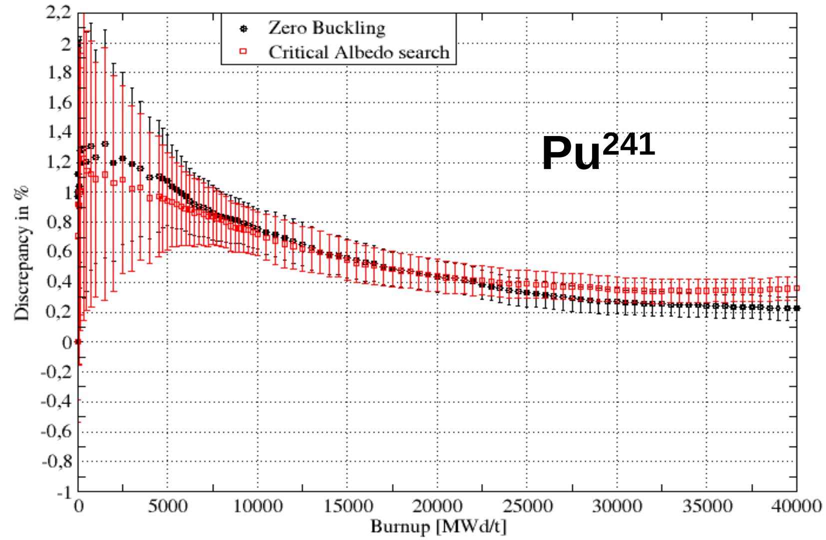
Reactivity discrepancies during irradiation (APOLLO2 vs TRIPOLI-4®)

DEPLETION CALCULATIONS: HEAVY ISOTOPES CONCENTRATIONS





- 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.



CONCLUSION AND PERSPECTIVE

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