# NEUTRONIC BEHAVIOR OF ATF CANDIDATES IN CANDU REACTORS

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*Abstract*

This paper evaluates the neutronic performance of several Accident Tolerant Fuel (ATF) concepts for CANDU reactors. Two approaches were considered: (i) $UO_2$ fuel pellets doped with metallic oxides and (ii) application of protective coatings on the fuel cladding. Three doped fuel variants were analyzed, all containing $Al_2O_3$ (Al/U = 0.02), with $Cr_2O_3$, $Nb_2O_5$, and $TiO_2$ as secondary dopants (0.16% metallic mass ratio). The cladding coating approach supposes the use of metallic chromium, FeCrAl alloy and CrN. Lattice calculations were performed using the DRAGON and WIMS computer codes to evaluate the infinite multiplication factor ($k_{inf}$) evolution with burnup, average discharge burnup (ADB), power distribution and coolant void reactivity (CVR). The results show similar behavior of ATF candidates to that of the standard CANDU fuel, but also some ADB penalties, which have been evaluated at core level using two distinct methods. In order to preserve the fuel cycle length, the initial fuel enrichment was reevaluated for the configuration with the highest ADB penalty. Safety-related parameters like power peaking factors (PPF), maximum channel and bundle power were comparatively presented and discussed.

***Keywords:*** *ATF, CANDU, DRAGON, core analyses*

## Introduction

The development of Accident Tolerant Fuels (ATF) is a major research direction in nuclear engineering, as response to the need for improving reactor safety after the Fukushima Daiichi nuclear disaster, which exposed the limitations of conventional uranium dioxide fuel and zirconium-based cladding under severe conditions.

ATF aims to enhance fuel performance during accidents without affecting normal operation. Key approaches include modifying the fuel composition (e.g., doping or alternative materials) and developing advanced cladding such as FeCrAl alloys or ceramic materials like CrN, to improve oxidation resistance, reduce hydrogen generation, and increase high-temperature stability, [1].

Originally developed for light water reactors (LWRs), ATF concepts are now being also considered for CANDU (CANada Deuterium Uranium) reactors, where specific neutronic characteristics require careful assessment of their impact on reactivity and burnup, [2]. In this respect, the present work aims to perform a neutronic analysis in order to assess the impact of implementing ATF concepts on fuel performance. The study considers two main development approaches. The first approach focuses on modifying the fuel pellet composition by doping uranium dioxide with aluminum, chromium, niobium, and titanium oxides, with the objective of improving thermo-physical properties and performance under accident conditions. The second approach consists of strengthening the cladding materials by applying additional coatings, as metallic chromium, FeCrAl alloy, and ceramic material like CrN, with the aim of increasing oxidation resistance and limiting degradation under high-temperature conditions.

## Fuel channel and core description

This study considers a CANDU 600 heavy water reactor operating with natural uranium (NU) fuel. The reactor vessel is cylindrical and accommodates 380 horizontal fuel channels oriented along the Z-axis, arranged in a square lattice with a pitch of 28.575 cm. The primary coolant circulates through adjacent channels in opposite directions, following a checkerboard flow configuration. Figure 1 illustrates the radial and axial view of the reactor core.

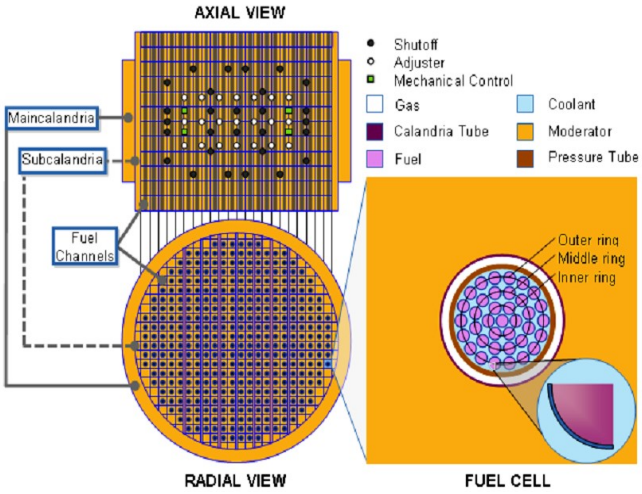



Fig. 1. Full-core CANDU-6 configuration, [3]

Under nominal operating conditions, on-power refuelling is carried out using two fuelling machines attached at both ends of a fuel channel containing 12 identical fuel bundles, each 49.53 cm long. The machine at the inlet (front end) inserts fresh bundles, while the one at the outlet (rear end) simultaneously removes the irradiated fuel. Figure 2 depicts the standard refueling pattern, which consists of an 8-bundle shift.

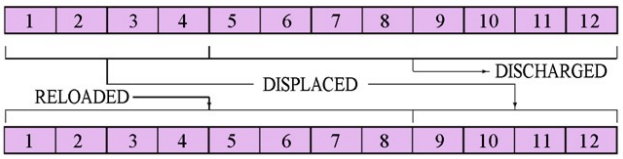



Fig. 2. Fuel Channel refueling scheme

Each lattice cell is defined as a Cartesian region filled with cold heavy water ($D_2O$) as moderator, that surrounds the calandria tube. A gas annulus provides thermal insulation between the calandria tube and moderator, and the high-temperature $D_2O$ coolant flowing within the pressure tube. The reference 37-element CANDU fuel bundle geometry is presented in Figure 3.

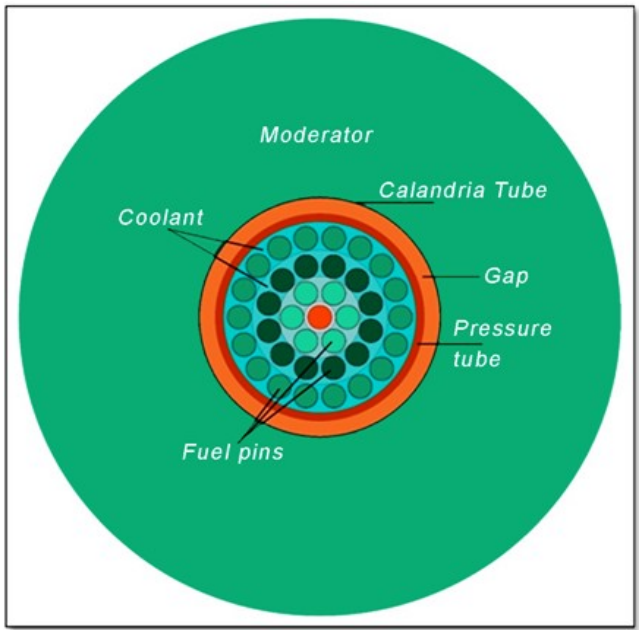



Fig. 3. Geometry of the standard 37-Element CANDU fuel bundle, lattice cell level (DRAGON plot)

**Modeling methodology**

Cell burnup calculations were performed using the transport codes WIMS [4] and DRAGON [5]. Both codes are using nuclear data from a 172 energy groups library based on ENDF/B-VII, provided by the International Atomic Energy Agency [6]. The simulated geometry consists in a 3D lattice cell model which is representative for the average CANDU 6 core. The radial section for this fuel bundle model is shown in Figure 3. The calandria tube and pressure tube are modeled using Zircaloy-2 and Zr–Nb alloys, respectively. The annular gap between the pressure tube and the calandria tube is filled with carbon dioxide, serving as an insulating medium. The heavy water ($D_2O$) coolant and moderator have different isotopic purities, with 97.5% for the coolant and 99.9% for the moderator. The coolant flows inside the pressure tube, while the moderator is outside the calandria tube. The model characteristics, as well as the material compositions and geometric parameters of the CANDU 6 fuel bundle, are based on a benchmark test problem presented in [7].

The cross section table sets generated by lattice calculations were introduced one by one in a standard CANDU 6 core model [8], and then adapted to the input of a 3D finite differences diffusion program, DIREN [9]. DIREN has been developed in RATEN ICN and is used to perform core burnup calculations in the time average (TA) approximation [10], along with Core Follow Simulations (CFS), which explicitly accounts for refueling operations, as shown in [8]. Apart from the channel and bundle power distributions, the DIREN program also provides an Average Discharge Burnup (ADB) value for the reactor core, which might be subject of penalties imposed by the use of dopants and considering clad coating options. These penalties are evaluated and discussed.

**Investigated fuels and working configurations**

Accident-tolerant fuel bundles were analyzed from two distinct perspectives: the first approach concerns the use of fuel pellets doped with various types of oxides, while the second refers to the addition of a supplementary coating applied to the cladding of the fuel elements. Three doped fuel variants are considered as presented in Table 1. Aluminum oxide is present in all three pellet fuel configurations, with a metallic mass ratio of Al/U equal to 0.02 wt%. As secondary dopants, chromium oxide, niobium oxide, or titanium oxide were used, each with a metallic mass ratio of 0.16 wt%.

Table 1. Working Configurations and Fuel Characteristics

| **Configuration** | **1** | **2** | **3** | **4** | **5** | ***6*** | **7** |
|---|---|---|---|---|---|---|---|
| Acronym | Ref. | Nb | Cr | Ti | +10μmCr | +60μmFeCrAl | +5μmCrN |
| Fuel matrix | $UO_2$ | $UO_2$ | $UO_2$ | $UO_2$ | $UO_2$ | $SEUO_2$ | $UO_2$ |
| Enrichment (%U235) | 0.711 | 0.711 | 0.711 | 0.711 | 0.711 | **0.767** | 0.711 |
| Aditive oxide | - | $Nb_2O_5$, | $Cr_2O_3$ | $Ti_2O_3$ | - | - | - |
| Metal/Uraniu (wt%) | - | 0.16 | 0.16 | 0.16 | - | - | - |
| Clad+Coating Material | Zry-4 | Zry-4 | Zry-4 | Zry-4 | Zry-4 + Cr | Zry-4 + FeCrAl | Zry-4 + CrN |
| Coating Thickness (μm) | - | - | - | - | 10 | 60 | 5 |
| Fuel density (% of TD of $UO_2$) | 96.7 [11] | 98.5 [11] | 98.2 [11] | 98.7 [11] | 96.7 [12] | 96.7 [12] | 96.7 [12] |

For the supplementary coating applied to the fuel element cladding, three materials were investigated: metallic chromium, an iron–chromium–aluminum (FeCrAl) alloy and chromium nitride (CrN) (see Table 1). The coatings were applied at recommended optimal thicknesses to ensure their effectiveness: 10 µm for chromium, 60 µm for the FeCrAl alloy, and 5 µm for CrN, [13, 14].

## Results and discussions

### Criticality evolution

The suggested fuels have been loaded homogenously into the CANDU-6 fuel bundle in independent fuel cycles, considering the same operation conditions.

For the fuels under investigation, the average power per bundle was 452 kW. Figure 4 presents the variation of the infinite multiplication factor $k_{inf}$ as a function of burnup for the two ATF bundle concepts under investigation.

As can be observed, both cases exhibit a similar behavior, characterized by an initial sharp decrease in $k_{inf}$, primarily due to the buildup of fission products with large neutron absorption cross sections (e.g., Xenon). This is followed by a subsequent increase reaching a maximum value, commonly referred to as the "plutonium peak" resulting from the combined effects of $^{235}U$ depletion and $^{239}Pu$ generation. At higher burnup levels, as fissile material is progressively depleted and fission products accumulate, a monotonic decline in $k_{inf}$ can be observed.

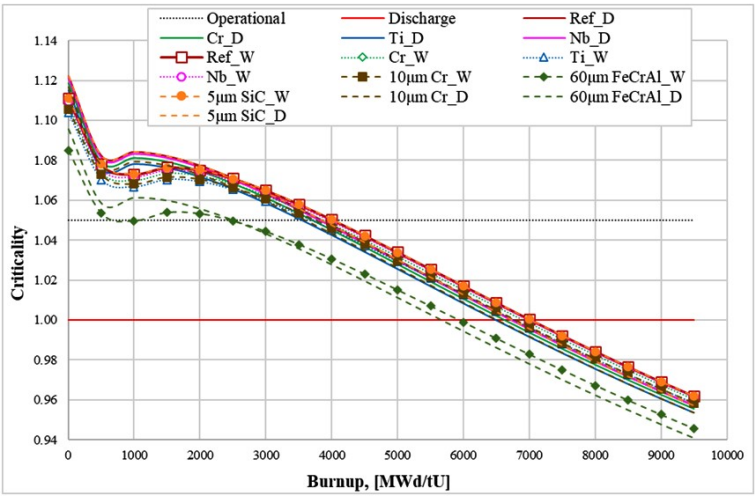



Fig. 4. Evolution of criticality for ATF cladding coated fuel bundles and the reference bundle

$Nb_2O_3$ doping preserves $k_{inf}$ values near to the reference throughout the entire burnup range, indicating a negligible neutronic penalty. In contrast, $Cr_2O_3$ introduces more reactivity degradation, while $TiO_2$ reduces $k_{inf}$ more significantly, particularly at higher burnup levels. For the coated ATF fuel bundles, the most significant neutronic penalties are observed in the case of FeCrAl coating, due to its larger effective thickness (60 µm). Regarding the lattice codes results, it should be mentioned that WIMS systematically provides greater values, by about 4%, compared to those of DRAGON, suggesting a consistent methodological bias between the two neutron transport-based approaches. Overall, $Nb_2O_3$ doping emerges as the most attractive option for reactivity preservation, whereas the additional FeCrAl coating layer leads to a substantial neutronic penalty, which might only be compensated by an increased enrichment of the fuel.

Another fuel performance parameter evaluated in this analysis was the maximum instantaneous critical burnup ($B_{max}$), which is the burnup value at which the cell is still critical, [8].

Table 2. $B_{max}$ values calculated using DRAGON and WIMS

| **Config. #** | **1** | **2** | **3** | **4** | **5** | **6** | **7** |
|---|---|---|---|---|---|---|---|
| Acronym | Ref. | Nb | Cr | Ti | +10µm Cr | +60µm FeCrAl | +5µm CrN |
| $B_{max}$ (MWd/kgU), WIMS Calc. | **7.02** | 6.99 | 6.91 | 6.77 | 6.79 | 5.93 | 6.91 |
| $B_{max}$ (MWd/kgU), DRAGON Calc. | **6.74** | 6.72 | 6.63 | 6.50 | 6.51 | 5.66 | 6.63 |

$B_{max}$ value for the CANDU standard fuel is taken as the reference, and the differences shown by ATF designs reflect the neutronic penalty induced by the dopants and clad coating. In the case of doping, $TiO_2$ leads to the largest reduction in peak burnup, $Cr_2O_3$ has a moderate effect, while $Nb_2O_3$ maintains values close to the reference, indicating low parasitic absorption. For cladding coatings, the effect is more pronounced: Cr introduces a limited penalty, FeCrAl results in the largest burnup reduction due to its consistent thickness, while CrN has a moderate impact, similar to that of Config. #3. The trends are consistent between WIMS and DRAGON.

A uniform power distribution throughout the bundle rings is considered a key feature for a good fuel performance and to prevent fuel sheath failure, but this is only ideal situation. In this respect, PPF is a measure of power uniformity inside the fuel bundle, being defined as the ratio between the mean linear power on the ring *i* ($Plin_i$) and the mean linear power on the bundle, $Plin_{bundle}$:

$$PPF_i = Plin_i / Plin_{bundle} \quad (1)$$

If all the PPF are close to 1.0, the power yield is evenly distributed across the bundle this indicating a uniform radial power distribution. The PPFs were calculated for all bundles at the beginning of cycle (BOL, B = 0) as well as for the fuel ready to be discharged, at the end of cycle (EOL, B = $B_{max}$). For the reference fuel bundles, PPF1, PPF2 and PPF3 are less than 1, while PPF4 is about 1.12.

As it can be seen in Figure 5, using ATF fuel bundles instead of the standard NU ones doesn't change significantly the radial power distribution. However, an easy reduction of PPF4 may be noticed at the BOL for all the fuel designs.

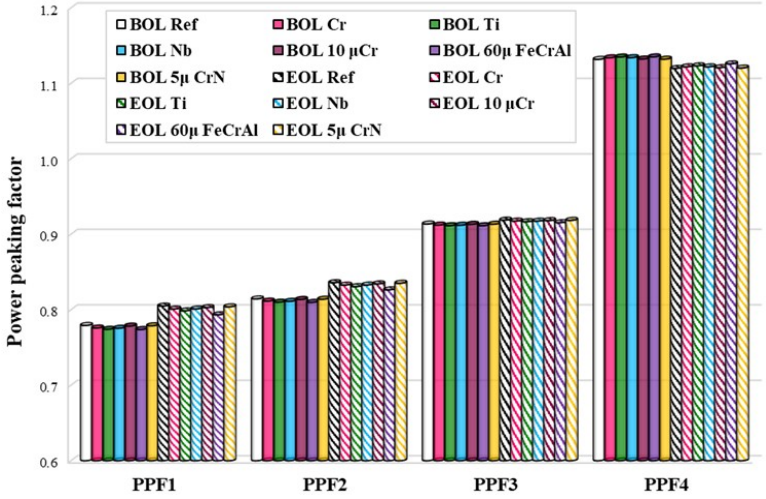



Fig. 5. WIMS estimation of power peaking factor at maximum burnup

The Coolant Void Reactivity (CVR) was treated as an instantaneous perturbation, and its evaluation was performed using a homogeneous approximation, in which the overall coolant density is reduced according to the void fraction (expressed in %), respectively *fv*=99% (see Eq.2). CVR for a given void fraction is then estimated as in Eq.3.

$$dens_{fv} = dens_0 \cdot \left(1 - \frac{fv}{100}\right) \quad (2)$$

$$CVR(fv) = \left(\frac{1}{k_{ref}} - \frac{1}{k_{fv}}\right) \times 1000 \quad (3)$$

The reference bundle ($UO_2$) yields CVR values of 15.2 mk (DRAGON estimation) and 16.7 mk (WIMS estimation) under fresh fuel conditions, decreasing to 10.7 mk and 11.9 mk, respectively, at BOL. This burnup-dependent behavior is consistent with values available in the literature [16, 17].

As shown in Figure 6, ATF fuel bundles exhibit CVR values comparable to the reference configuration for both fresh and irradiated fuel conditions.

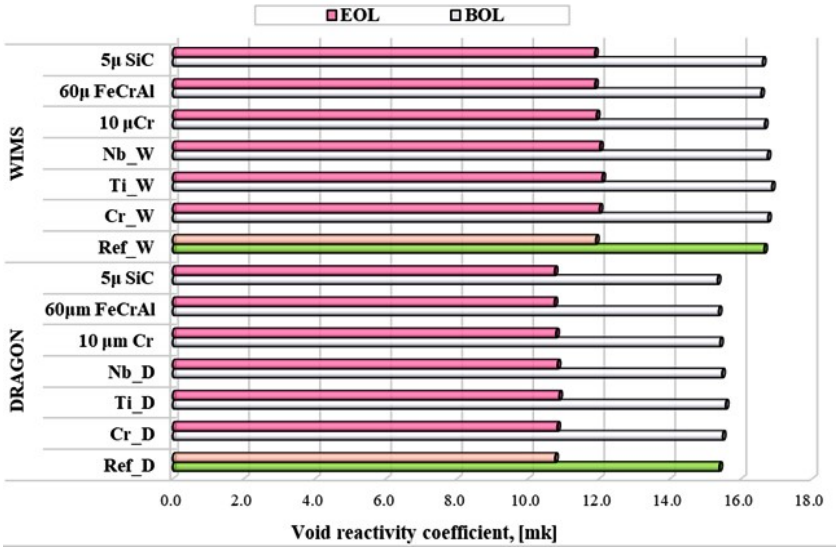



Fig. 6. Void reactivity coefficient at BOL and EOL

Doped ATF concepts yield a slight increase relative to the reference case (0.6–1.3%), whereas coated-cladding designs show marginally lower values, with reductions that not exceeding 0.5%, as observed for the FeCrAl case.

**Core calculation results**

The time average core calculation result are shown in Table 3, in form of relevant integral parameters as: maximum channel and bundle powers, radial form factor (RRF), discharge burnup (ADB), dwell time, fuel bundle consumption, maximum channel and bundle powers, and burnup penalties. RFF is a measure of power flattening over the reactor core, it being the ratio between the average and maximum channel powers and should be as close as possible to unity. A typical value reported for a CANDU 6 unit is 0.83, [18].

Table 3. Core time average results

| **Config. #** | **1** | **2** | **3** | **4** | **5** | **6** | **7** |
|---|---|---|---|---|---|---|---|
| Acronym | Ref. | Nb | Cr | Ti | +20 μmCr | +60μm FeCrAl | +5μm CrN |
| Maximum channel power (kW) | **6484** | 6487 | 6486 | 6509 | 6505 | 6658 | 6494 |
| Maximum bundle power (kW) | **788** | 789 | 787 | 786 | 788 | 773 | 789 |
| Radial Form Factor | **0.84** | 0.84 | 0.84 | 0.83 | 0.83 | 0.81 | 0.84 |
| Uranium mass per bundle (kg) | **19.0** | 18.95 | 18.95 | 18.95 | 19.0 | 27.5 | 19.0 |
| Dwell time (FPD*) | **206** | 204 | 198 | 187 | 189 | 110 | 197 |
| Fuel consumption (bundles/FPD) | **14.7** | 14.9 | 15.4 | 16.2 | 16.1 | 27.5 | 15.4 |
| ADB (MWd/kgU) | **7.42** | 7.35 | 7.11 | 6.73 | 6.79 | 3.98 | 7.11 |
| Absolute penalty (MWd/kgU) | - | -0.07 | -0.31 | -0.69 | -0.63 | -3.4 | -0.03 |
| Relative penalty (%) | - | -0.9 | -4.1 | -9.2 | -8.5 | -45.0 | -4.1 |

* FPD = Full Power Days

The safety core integral parameters have similar and close values (maximum channel and bundle powers, RFF and core reactivity) for the majority of designs. This means that all the configurations allow for operation in a similar manner. Differences appear when economic parameters like dwell time and ADB are extracted. The dwell time is the time when the average channel is expected to be refuelled, due to exhausting the initial fresh fuel reactivity excess. The concept of average channel is specific to the time average (TA) approximation, its neutronic properties being an average over the reactor core weighted by the target exit irradiation. A typical TA CANDU 6 dwell time value is near to 200 Full Power Days (FPD), [19].

According to the dopant absorption strengthening, the initial reactivity excess is more and more rapidly exhausted and the average fuel channel must be refuelled earlier and earlier, increasing the bundle consumption and worsening the ADB. Thus, the most severe consequence take place in the case of FeCrAl coating design, where dwell time is shortened to about a half of the reference value. Accordingly, the fuel consumption (bundles/FPD) increases twice, from 14.7 to to 27.5 bundles/FPD. It is clear that such an economic penalty cannot be accepted by the Nuclear Power Plant (NPP) owner. Considering that an ADB penalty larger than 10% is not acceptable and seeing good safety behavior during operation, all ATF designs (excepting FeCrAl one) might be use “as is” in actual CANDU reactor without the need for enrichment. If a more robust ATF design (as FeCrAl coating, for example) is desired, then the fuel enrichment cannot be avoided.

In this respect, a series of CFS calculations, well documented in [8], have also been performed for all configurations of Table 1, excepting the sixth (FeCrAl coating), where an equivalent enrichment of only 0.767% $^{235}U$ (instead of 0.711%) was used, to preserve the fuel cycle length. The CFS results are shown in Table 4.

The CFS results are generally in good agreement with those of the TA approximation, with one exception: the fuel doped with titanium oxide provided a significantly lower ADB (by 19%) than the standard fuel design. This also means, as in the case of FeCrAl coating, that using titanium as a dopant without some enrichment of the standard fuel is not sustainable on long term operation of the nuclear unit.

Table 4. CFS results

| **Config. #** | **1** | **2** | **3** | **4** | **5** | **6** | **7** |
|---|---|---|---|---|---|---|---|
| Acronym | NU (Ref.) | Nb | Cr | Ti | +20μmCr | +60μmFeCrAl | +5μmCrN |
| Maximum channel power (kW) | **7083** | 7088 | 7097 | 7099 | 7098 | 7099 | 7096 |
| Maximum bundle power (kW) | **910** | 910 | 885 | 881 | 883 | 901 | 902 |
| Fuel consumption (bundles/FPD) | **14.7** | 15.1 | 15.9 | 18.2 | 16.3 | 14.9 | 16.2 |
| ADB (MWd/kgU) | **7.34** | 7.18 | 6.81 | 5.95 | 6.67 | 7.30 | 6.74 |
| Absolute penalty (MWd/kgU) | - | -0.16 | -0.53 | -1.39 | -0.67 | -0.04 | -0.6 |
| Relative penalty (%) | - | -2.1 | -7.2 | -18.9 | -9.2 | -0.54 | -8.2 |

## Conclusions

A comparative analysis of the neutronic performance of ATF bundles in a CANDU-6 reactor using the WIMS, DRAGON and DIREN programs has been performed. The study focused on the evolution of relevant lattice and core neutronic parameters with respect to the burnup for several ATF concepts, compared to the standard natural uranium fuel-zircaloy cladding system. The results highlight the effect of fuel doping and cladding modifications on key neutronic parameters.

The analysis of the main neutronic parameter, namely the maximum discharge burnup, indicates that the ATF concepts have a significant impact on fuel economics, as follows: $TiO_2$ reduces burnup the most, $Cr_2O_3$ exhibits a moderate effect, while $Nb_2O_3$ remains close to the standard $UO_2$ fuel, taken as a reference. For cladding coatings, FeCrAl leads to the most significant decrease and requires enrichment, while Cr and CrN have a limited impact.

The use of ATF bundles has no major effect on power flattening inside the fuel bundle, as all the pairs of PPF have similar values, which are close to those of the reference design.

Both lattice transport codes used in analysis indicate that the implementation of ATF concepts has a negligible impact on the CVR.

Formally, considering that an ADB penalty greater than 10% is unacceptable and seeing appropriate safety behavior during operation, all ATF designs (excepting titanium doping and FeCrAl coating) could be used "as is" in actual CANDU reactors, without enrichment. If a more robust ATF design is desired, the fuel enrichment is mandatory.

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