



# Application of the GRS core simulator KMACS on Accident Tolerant Fuels

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## 1. Introduction

The nuclear simulation chain of GRS comprises well-established tools in the field of nuclear safety analysis [1]. The core simulator KMACS, as part of the GRS calculation tools, is used and validated for standard light water reactor (LWR) fuel compositions, e.g.  $\text{UO}_2/\text{Zr-4}$  [2]. In this work we want to explore the potential of KMACS in terms of its applicability on *Accident Tolerant Fuels* (ATF). ATF are recently studied innovative fuel materials with improved robustness under severe accident conditions [4]. In ATF, well-established fuel components are complemented or replaced by different, new materials, and thereby adding elements such as iron, chromium, aluminum, silicon, or carbon to the set-up. These modifications will not only have an influence on the thermo-mechanical, but also on the neutronic properties of the system [3]. In this study, besides the standard combination  $\text{UO}_2/\text{Zr-4}$  as reference case, we selected two ATF concepts for further investigation: the standard combination with an additional chromium coating,  $\text{UO}_2/\text{Zr-4}/\text{Cr}$ , and a combination with uranium dioxide as fuel material and an iron-chromium-aluminum cladding,  $\text{UO}_2/\text{FeCrAl}$ .

## 2. Methodology

The calculations performed in this study comprise criticality calculations of single assemblies in an infinite lattice, the determination of few-group cross-sections, nodal flux calculations for the whole core as well as a cycle calculation for an operating cycle.

The models are based on the specification of the first operating cycle of the BEAVRS benchmark [5]. The reactor considered in this benchmark is a four-loop Westinghouse PWR loaded with 193 fuel assemblies. A special characteristic of this core are the additional neutron shield panels at the corners of the core. The original core is loaded with fresh  $\text{UO}_2$  fuel assemblies with different enrichments, 1.6%, 2.4% and 3.1% U-235. First, on basis of the 3.1% U-235 assembly, we perform criticality calculations of the single assembly in an infinite lattice. Thereby, the original fuel cladding is exchanged with the ATF cladding materials. The applied codes are SCALE 6.2.3/T-NEWT [9] with the 56-group cross section library based on ENDF/B-VII.1 shipped with SCALE, and HELIOS-2 [6]. The corresponding inputs for the calculations are generated as well as triggered by KMACS. Independent Monte Carlo reference calculations are performed using Serpent [8] with the continuous energy (CE) library based on ENDF/B-VII.0. As next step, we perform whole-core calculations under HZP conditions using the modified BEAVRS core. Thereby, we only consider the ATF-material  $\text{UO}_2/\text{FeCrAl}$ . In total we exchange 32 fuel assemblies of the 3.1% U-235 type, which are located at the outermost part of the core. The homogenized two-group cross-sections are generated using SCALE 6.2.3/T-NEWT and as nodal flux solver QUABOX/CUBBOX (Q/C) [7] is applied. Again, KMACS is used to orchestrate the input generation, calculation execution, and the post-processing of the results. The

reference solution is obtained with the Monte Carlo code Serpent.

Further, we conduct an operating cycle calculation for the first cycle of the BEAVRS benchmark. Analogously to the HZP calculation before, 32 fuel assemblies are exchanged with ATF assemblies. Two cases are considered: the unmodified core with standard  $\text{UO}_2/\text{Zr-4}$  fuel assemblies, and the modified core with  $\text{UO}_2/\text{FeCrAl}$  assemblies. The homogenized cross-sections for branched operating conditions of the reactor are generated using SCALE 6.2.3/T-NEWT. Based on these cross-sections, the whole-core calculation is performed with the coupled neutron-kinetic/thermal-hydraulic code system Q/C-ATHLET [7].

### 3. Results and Discussion

The multiplication factors obtained in the single assembly calculations with SCALE 6.2.3/T-NEWT and HELIOS-2 are compared with Serpent reference calculations. We observe reactivity differences up to 389 pcm (cf. Table I), which lay in a typical range of such comparisons.

Table I: Neutron multiplication factor for unirradiated fuel assemblies.

Case	SCALE/T-NEWT	HELIOS-2	Serpent CE
$\text{UO}_2/\text{Zr-4}$ (ref.)	1.27265	1.27244	1.27742
$\text{UO}_2/\text{Zr-4}/\text{Cr}$	1.25605	—	1.26222
$\text{UO}_2/\text{FeCrAl}$	1.16054	1.16302	1.16312

The Q/C nodal flux solution under HZP condition based on the few-group cross-sections is in good agreement with the Serpent reference solution in terms of the multiplication factor and the radial power distribution. As shown in Table II, we obtain a reactivity difference of 208 pcm, which is an acceptable deviation for such calculations.

Table II: Neutron multiplication factor of modified BEAVRS core under HZP conditions.

Case	SCALE/T-NEWT	Serpent CE
$\text{UO}_2/\text{FeCrAl}$	0.99027	0.99231

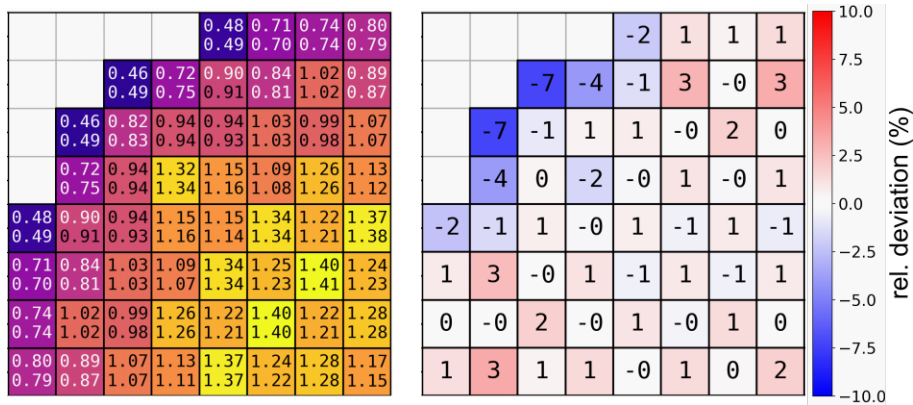


Figure 1: Radial power distribution (left) obtained from the Q/C (upper value) and Serpent (lower value) calculations and relative deviation of the radial power distribution (right) at BOC.

The radial power distribution and its deviation compared to the Serpent results are illustrated in Figure 1. The results show an overall good agreement with the Monte Carlo reference solution.

However, at the corner positions of the core we observe deviations up to 7%. These deviations are probably caused by the additional neutron shield panels (cf. BEAVRS specification [5]), that are not well captured by our nodal whole-core model.

In Figure 2, the boron curves of the original case with the  $\text{UO}_2/\text{Zr-4}$  assemblies and the modified case with  $\text{UO}_2/\text{FeCrAl}$  assemblies resulting from the cycle calculations with Q/C-ATHLET are shown. For comparison, also the measured boron curve from the benchmark specification which refers to the original core is shown. Due to the higher neutron absorption of the ATF cladding material FeCrAl in comparison to the original Zr-4 cladding material, the corresponding boron curve lies below the original case. Caused by the in general lower boron concentration, the natural cycle end is already reached after approximately 280 EFPD for the ATF-modified case. Afterwards, Q/C-ATHLET tries to keep the critical state by introducing a negative boron concentration. Physically, this makes no sense, but can be considered as numerical artifact.

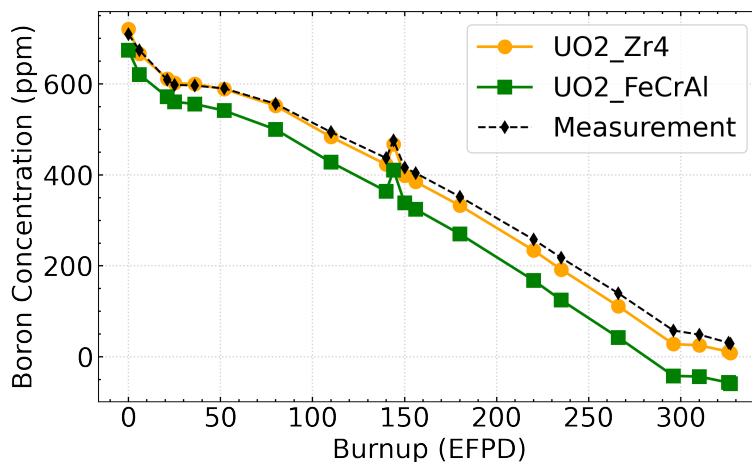


Figure 2: Boron curve of cycle 1 for the reference core loading and the core partially loaded with ATF assemblies and the measurement.

#### 4. Conclusions

The work presented here shows the applicability of the GRS core simulator KMACS on modern ATF materials for LWR applications. Thereby, criticality calculations for fresh fuel, the generation of homogenized two-group cross sections, and the whole-core calculations for the HZP state as well as for the full operating cycle are performed successfully. The criticality calculations as well as the whole-core calculation under HZP conditions show good agreement with the reference Monte Carlo calculations. In case of the cycle calculation, the observed lower boron concentration of the core partially loaded with the ATF assemblies is physically plausible. Only the modeling of fuel assemblies with an additional coating layer (e.g.  $\text{UO}_2/\text{Zr-4}/\text{Cr}$ ) needs to be revised in KMACS. Although HELIOS-2 and ATHLET are in principle able to model additional coating layers, KMACS does not support the generation of the corresponding inputs for these codes. However, this problem will be solved in the near future. Currently, also the GRS fuel behavior code TESP-ROD [10] is upgraded to analyze FeCrAl cladding systems and will be linked to the KMACS system.

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## References

- [1] A. Schaffrath, A. Wielenberg, M. Sonnenkalb, R. Kilger, “The nuclear simulation chain of GRS and its improvements for new ALWR and SMR typical phenomena”, *Proceedings of the Intl. Conf. 12th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics, Operation and Safety (NUTHOS-12)*, Qingdao, China, October 14-18, 2018, (2018).
- [2] M. Zilly, and Y. Périn, “KMACS Validation Report”, *Technical Report GRS-P-8/Vol. 2, Rev. 0*, Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) gGmbH (2018).
- [3] R. Kilger, and R. Henry, “Application of the Neutronic Part of the Nuclear Simulation Chain of GRS to Accident Tolerant Fuel Systems – First Results.”, *International Conference on Nuclear Criticality Safety (ICNC)*, Paris, 15-20 Sep 2019, vol. 52. (2019)
- [4] S. J. Zinkle, K. A. Terrani, J. C. Gehin, L. J. Ott, and L. L. Snead, “Accident tolerant fuels for LWRs: A perspective”, *Journal of Nuclear Materials*, vol. 448, pp. 374–379 (2014).
- [5] N. Horelik, B. Herman, M. Ellis, S. Kumar, J. Liang, B. Forget, K. Smith, “Benchmark for Evaluation And Validation of Reactor Simulations (BEAVRS)”, Release rev. 2.0.2. 177 S. (2018).
- [6] J. J. Casal, R. J. J. Stamm’ler, E. A. Villarino, A. A. Ferri, “HELIOS: Geometric Capabilities of a New Fuel-assembly Program”, *Proc. Int. Topl. Mtg. Advances in Mathematics, Computations, and Reactor Physics*, Pittsburgh, PA, USA, 28. April 1991, vol. 2, pp. 1-13 (1991).
- [7] S. Langenbuch, K. Velkov, “Overview on the Development and Application of the Coupled Code System ATHLET-QUABOX/CUBBOX”, *Proc. M&C 2005*, Avignon, France, September 12–15, 2005, American Nuclear Society (2005).
- [8] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, T. Kaltiaisenaho, “The Serpent Monte Carlo Code, Status, Development and Applications in 2013”, *Annals of Nuclear Energy*, 82, pp. 142–150 (2015).
- [9] B. T. Rearden, M. A. Jessee, *SCALE Code System, ORNL/TM-2005/39, Version 6.2.3*, Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee, USA (2018).
- [10] H.-G. Sonnenburg, F. Boldt, “Brennstabverhalten im Normalbetrieb, bei Störfällen und bei Langzeitlagerung”, *GRS-464, 108 S., DOI 10.2314/GBV:1011412691*, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH: Köln, Garching b. München, Berlin, Braunschweig, (2017).