SURROGATE-BASED OPTIMIZATION MODEL OF BEST-REPRESENTATIVITY SODIUM FAST REACTOR SEVERE CORE ACCIDENT REACTIVITY EFFECTS IN THE ZEPHYR CRITICAL FACILITY

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Abstract

This project deals with original representativity studies of local reactivity effects in a fast lattice during severe core accident in Sodium-cooled Fast Reactor aiming to implement new experimental programs in the French ZEPHYR project of new critical facility. This representativity study is based on sensitivity analysis of reactivity coefficients and local flux distribution in case of degradation of the ASTRID inner core. SCA sequence, e.g., voiding, fuel meltdown etc., potentially has pronounced influence on the neutronic characteristics of the fast reactor's core and can lead to prompt recriticality. To predict the core behavior during such disruptions, it is necessary to develop accurate and reliable computational and experimental tools and methodologies. The assessment of reactivity behavior that represents different stages of the disrupted core configurations is one of the challenges assigned to ZEPHYR and requires a new way of performing measurements in critical assemblies. The project is carried out in both assembly and core levels. Recent results indicate that it is possible to identify high representativity experimental configurations using surrogate-based approaches for a 2-step optimization strategy.

1. Introduction

Safety standards for nuclear reactors are a dynamic topic that is being influenced by global events, e.g., Three Mile Island, Chernobyl and Fukushima Daiichi [1]. Therefore, continuous research efforts concerning the safety of nuclear power plants are fundamental for the nuclear community. Although severe core accident (SCA) analysis and research have been performed through the evolution of nuclear systems, the entire range of possible scenarios is yet to be examined [2, 3]. Thus, adequate analyses are needed for all phases of SCA in order to fully understand the phenomena involved. The main knowledge gaps were identified by the EUROSAFE forum [4]. These gaps mainly related to mechanical, chemical, and material problems related to reactor behavior under SCA progression.
Naturally, the focus is on thermal reactors, where the SCA phases are somewhat well understood [5]. However, when considering SCA in GEN-IV future proposed systems [6], such as Sodium-cooled Fast Reactors (SFRs), it is strongly dependent on the neutronic characteristics of the core, since typically, Fast Reactors (FRs) are not loaded in their most critical configuration. Hence redistribution of different materials in the core, e.g., fuel, sodium, absorbers, or structural material has the potential to lead to unrestrained power excursion. Therefore, detailed neutronic characteristics of the core during SCA are an essential part of the studies related to core accidents in FRs. The reactivity of the core is affected by a wide range of reasons [7], such as loss of coolant, structural/fissile material relocation, and molten

pools formation. All those scenarios lead to core configuration modification and have a strong effect on the neutronic behavior of the core.
Accordingly, support of the analytical research efforts by experimental programs for core behavior studies during SCA is essential for the development of best estimate tools and instrumentation for SCA progression monitoring and mitigation. SCA is a non-coherent step-wise process, which can lead to many different outcomes, which require a quasi-analytic approach, at least to validate instantaneous critical situations during the meltdown sequence. The latter could be achieved through a dedicated experimental program for tool validation. Therefore, in order to provide the most relevant information to the investigated reactor (thermal or fast), the experiment design should be characterized as “Best Representative” [8, 9, 10]. Such experiments provide information according to the specification of the end-user on different physical quantities (e.g., reactivity, flux distribution) with respect to the experimental system, which can be transferred to the reference system.
The investment of the French scientific community in the ASTRID SFR industrial demonstrator targets the low sodium void fraction (CFV) of the ASTRID as the reference system that requires support by an experimental program for core physics validation [11], due to its axial heterogeneous layout. The behavior of the axial heterogeneity under severe accident scenarios, such as sodium voiding, compaction of the two fissile zones into two molten zones and compaction of the entire upper part of the core to a single mass, is of a great interest in the frame of the ASTRID SFR project.
The design of the “Best Representative” experimental program dedicated to the CFV type core is the main goal of the current project. The emphasis is put on the *temperature effects* occurring at ~3000^{o}C in the core and the way it can be represented in a Zero Power Reactor (ZPR). Two main parameters, temperature and material density, dominate the problem. The former affects both microscopic and macroscopic cross-sections, whereas the latter affects macroscopic cross-sections only. Considering these two direct influencers on the macroscopic cross-section, it is possible to define the main challenge – how does *reactivity temperature effects* in a power reactor are transferred to *reactivity density effects* in a zero-power reactor. The current study is a first-of-a-kind feasibility study, carried out in collaboration between CEA Cadarache and Ben-Gurion University of the Negev in the framework of the Zero-power Experimental PHYsics Reactor (ZEPHYR) project [12, 13] for SCA investigation.

2. Methodology

The challenge is addressed in two steps. First, the “Best Representative” configuration is identified on the assembly level. This enables a meticulous study of the parameter space and provides indications for the existence of representative solutions. Second, full core representative solutions are investigated, considering the effects from the surrounding of the degraded zone. The Serpent Monte Carlo code is utilized [14, 15] for this study.

2.1. Representativity

The representativity model is based on a method proposed by Orlov et al. [16]. Utilization of the representativity methodology in experiment design plays an important part in the safe design of future nuclear systems. Thus, a ZPR could be considered for neutronic modeling of relevant SCA configurations by ensuring high level of representativity of the examined system. When an *experimental* system ***represents*** an *examined* system, then physical quantities measured in the *experimental* system can be translated into analogous quantities in the *examined* system with only minor corrections. A measure for the quality of representativity between two systems is based on comparison of the sensitivity vectors of the same integral quantity. The representativity is linked to the definition of the correlation coefficient (noted as r_{RE}), and defined in Eq. 1

$$r_{RE} = \frac{\boldsymbol{S}_R^t \cdot \boldsymbol{V} \cdot \boldsymbol{S_E}}{\sqrt{\boldsymbol{S}_R^t \cdot \boldsymbol{V} \cdot \boldsymbol{S_R}} \cdot \sqrt{\boldsymbol{S}_E^t \cdot \boldsymbol{V} \cdot \boldsymbol{S_E}}} \tag{1}$$

where the subscripts $\boldsymbol{E}$ and $\boldsymbol{R}$ correspond to the experimental mock-up and the examined power system, respectively. $\boldsymbol{S}$ is the sensitivity vector of the examined integral quantity to perturbations in the nuclear data. $\boldsymbol{V}$ is the nuclear data variance-covariance matrix. In this work the COvariance MAtrix Cadarche (COMAC) V01 is utilized [17].
The ultimate goal of the project is to achieve the most representative configuration ($r_{RE} = 1$). A minimal threshold was set to $r_{RE} = 0.85$ which should suffice for representativity studies [18, 19, 20].

2.2. Optimization Strategy

The design process of a representative assembly is a six-step sequence and is valid for the two parts of the entire work. The steps are summarized below. As a versatile facility, fast lattices of the ZEPHYR project are based on the use of the MASURCA rodlets and plates stockpile [ref].
Step I – Calculate the SFR reference configuration and associated nuclear data sensitivity profiles at HFP conditions (around 900^{o}C).
Step II – First optimization step, to determine the most representative configuration for the ZEPHYR core, by modifying its layout in such manner that it reaches best representativity of the SFR core calculated in step I.
Step III – Calculate the SFR degraded configuration and its associated nuclear data sensitivity profiles at target temperature (in this work; the temperature varies from 1000-3000^{o}C).
Step IV – Second optimization step, to determine the optimal amount of PuO_2 in the MOX fuel that results in the best representative reactivity variation between the reference SFR core (steps I and III) and the ZEPHYR configuration (step II) loaded with degraded configuration in the core center .
Step V – Select fuel plates available in the MASURCA ZPR stockpile to correspond as close as possible to the parameters found in step IV.
Step IV – Recompute the "actual" representativity, based on the actual available stockpile.
The search space of the different parameters such as geometry and material content is huge. It is practically impossible to traverse it, especially with the utilization of Monte Carlo code for full core calculations. The single fuel assembly calculations are less costly in Monte Carlo codes and serve in this project as concept validation and provide initial guess for the core step.

2.2.1. Optimization strategy for Assembly level

When a single fuel assembly is considered, it is possible (computationally-wise) to examine the influence of a wide range of parameters on the representativity. In order to achieve this goal, the Particle Swarm Optimization (PSO) [21] is selected as an efficient optimization approach.
The PSO is a swarm intelligence metaheuristic, which was inspired by the flocking behavior of animals (i.e., birds, fish). The PSO is a population-based method, which is composed of individual solutions with different fitness. The population of the PSO is iterated until some termination criterion is satisfied. The population, $P = \{p_k\}_{k=1}^{n}$, is often addressed as "the swarm" and is consisted of n single solutions, p_k, (also known as "particles") located in the search space. Each particle integration is made by updating its position by the "velocity", which determines the direction and the intensity with which it travels in the search space. The velocity is divided into three main components – Personal Inertia, Social and Personal impacts. The personal inertia represents the impact of previous iteration velocity on the subsequent direction of the particle. Each particle in the swarm contains two types of information; personal, corresponding to the best solution obtained by the particle so far, and social, corresponding to the best position obtained by the entire swarm in the entire simulation. Thus, the movement of the particle is dictated by the distance between the current location and the personal and social best solutions.
In the current study, the particle of the PSO are subjected to predefined constraints (i.e., content of PuO_2 in the MOX fuel or specific zone geometrical parameters) and are iterated by

executing the Monte Carlo code Serpent 2 for obtaining the sensitivity profiles [15], followed by evaluation of the representativity factor for each particle. After the evaluation of the representativity factor, the particle is updated with respect to the particle's self-best and the entire swarm's best results. The flow chart of the PSO is shown in Fig 1.

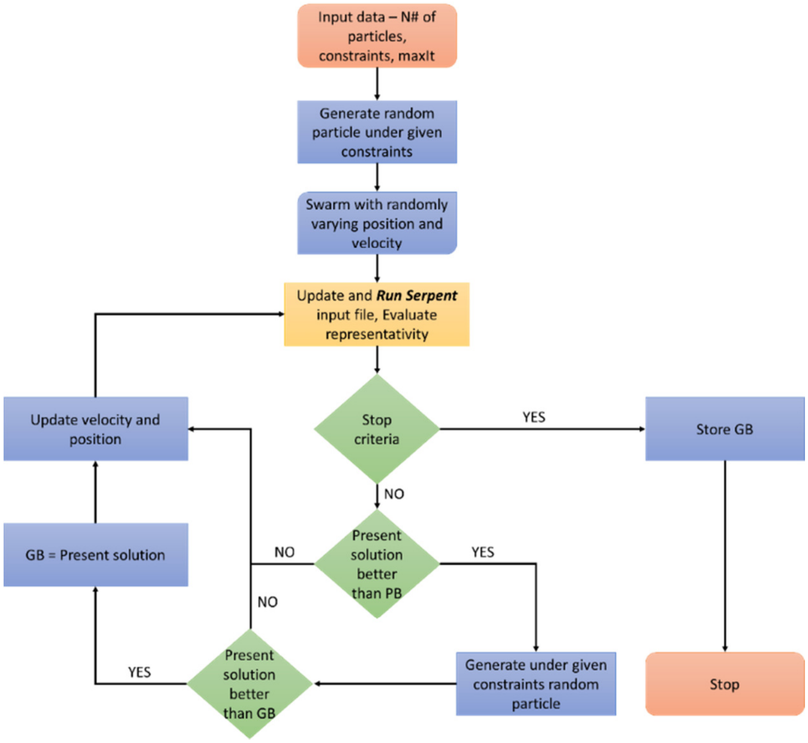


Fig 1. PSO algorithm for global maximum search of a given representativity problem

2.2.2. Optimization strategy for Core level

On the other hand, the optimization of the core requires a different approach. In comparison to the assembly level, full core calculation requires much more computational resources. Therefore, a population-based optimization is impractical. Considering the relatively smooth behavior of the representativity over the search space in the single fuel assembly case, the Nelder-Mead Downhill Simplex Method (NM) [22] is selected for the core optimization.

3. Examined configuration

The ASTRID industrial demonstrator is designed to answer all the requirements set by the GEN-IV forum [6]. In this study, the focus is made on the ASTRID low void fraction V0 core configuration, with several accidental scenarios already investigated [11]. The CFV-V0 core is a 1500 MWth full power reactor, with PuO_2 content in the MOX of about 22.8% in all the fissile zones. The core consists of two axial fissile zones (lower/upper) of about 25/35 cm long.

SCA can develop into different scenarios. In the case of the CFV-V0 core configuration several SCA scenarios are drawing more attention and require investigation due to the heterogeneous axial arrangement of the fuel assembly, as show in Fig 3. In the current study, the leading initiator event of the SCA is assumed to be a total instantaneous blockage of the central seven fuel assemblies, which are then geometrically modified according to cases 'a', 'b' and 'c' in Fig 3. Case 'a' – total voiding of sodium, Case 'b' – compaction of the two fissile and the intermediate fertile zones in to a single molten mass, and Case 'c' – compaction of each of the axial fissile zones separately.

At this stage of research, it is assumed that the sodium voiding expands to the upper sodium plenum as well. This allows some simplifications to the optimization process by concentrating on the fuel compaction effects and neglecting neutron reflection from the sodium plenum.

Thus, the study concentrates on the 110 cm of the fertile and fissile zone excluding the sodium plenum which would require the modeling of 200-250 cm.

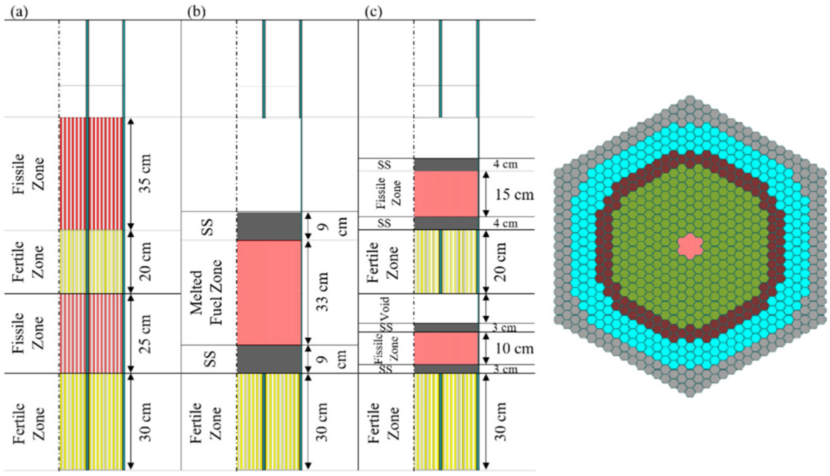
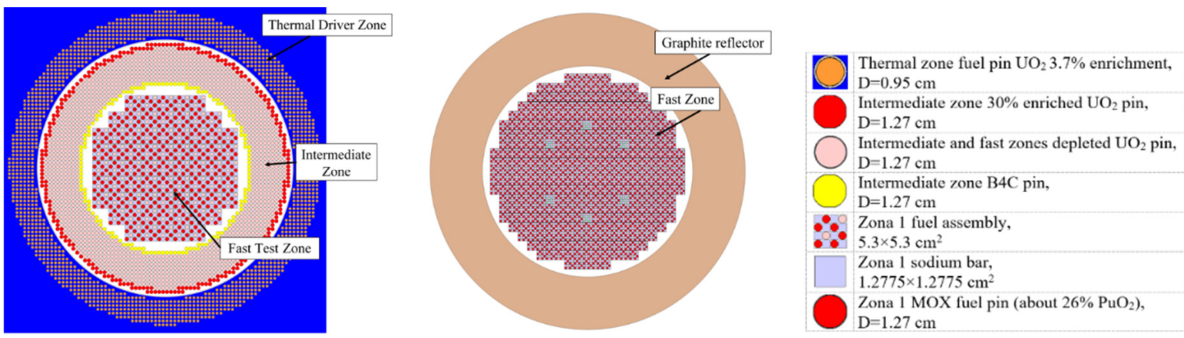


Fig 3. ASTRID degraded configuration.

The above assumption enables to avoid possible fuel assembly scaling problems resulting from incorrect representation of the leakage in the ASTRID configuration due to ZEPHYR fuel assembly restriction of 90 cm fixed height.

Preliminary examination of the ZEPHYR coupled fast/thermal (Fig 4a) characteristics show that it is impossible to achieve high representativity values [23] due to a large flux perturbation that reaches the thermal zone, in the case of single fuel assembly modification. This prevents the vanishing of the sensitivity coefficients of ^{235}U, which become the main contributor to the low representativity since the ASTRID core contain very low quantity of ^{235}U. Therefore, a modification to the ZEPHYR core is proposed and a full fast core is foreseen for the new facility (Fig 4b).

The degraded geometries to be loaded into the ZEPHYR are shown in Fig 6. The configurations are similar to the ASTRID examined configurations (Fig 4), i.e., sodium voiding, single compacted zone and two compacted regions. Preliminary studies [23] show that the optimization converges faster when the relative heights are conserved as in the ASTRID configurations. Thus, the search is performed on the amount of PuO_2 in each zone, with a constant plutonium vector dictated by the MASURCA stockpile.



(a) Coupled fast/thermal (b) Fast (c) legend

Fig 4. ZEPHYR possible configurations

4. Results and discussion

The results in this section provide an overview of the optimization made on the assembly level (PSO optimization). Results on the core level will be published elsewhere. The reference assembly level configuration, from which reactivity variation is calculated, is the sodium voiding (Fig 3a for the ASTRID and Fig 5a for the ZEPHYR). Each optimization step starts with the k_{eff}-representativity evaluation of the reference configuration, followed by the representativity of the reactivity variation.

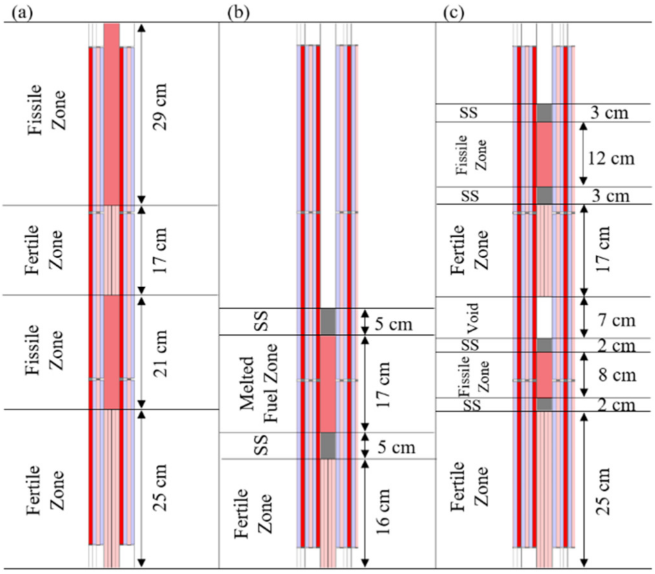


Fig 5. Degraded configurations for the ZEPHYR reactor – axial cross section

4.1. Fuel assembly optimization

The time required for a fuel assembly calculation is relatively short thanks to both Serpent code capabilities and the computational resources available on Ben-Gurion University HPC cluster. This allows for a deeper study on the effects of temperature on the representativity process. Therefore, the simulation of the fuel assembly is performed according to both the classical approach to criticality representativity, where both systems are set at 20°C, and to a more realistic approach, where the examined system is set at 900°C and the experimental is at 20°C. The same dual-approach method is implemented for the reactivity variation representativity. The temperature variations considered in this step are 20°C/20°C, 900°C/1000°C, 900°C/2000°C and 900°C/3000°C, where the first temperature corresponds to the temperature of the reference configuration and the second temperate corresponds to the degraded configuration.

The first step criticality representativity results are summarized in Table 1, for the representativity of the reference ASTRID configuration multiplication factor. The results show that there is a possibility to reach high representativity values of the multiplication factor for the different temperatures, with different content of PuO_2 in the MOX. The temperature impact is visible, where less PuO_2 is required for the same level of representativity at the two examined temperatures. However, an interesting observation is made when the COMAC matrix is replaced to the Updated COvariance Matrix V01AB (UCOM - updated version of COMAC with reduced uncertainties [24]). The representativity drops in about 3%, and the content of the PuO_2 is increased. This change occurs due to a shift in the isotopic importance in the representativity optimization process and the difference in the fuels of the two systems, mainly the plutonium vector of the two systems. When COMAC-V01 is utilized, the main isotopes contributing to the representativity are ^{238}U and ^{239}Pu, as being materials with the highest uncertainties and abundance in the two systems. However, UCOM-V01AB targeted the two isotopes' uncertainties (were reduced by 50%) and hence the importance of the two dropped, increasing the importance of ^{240}Pu. The ^{240}Pu content varies strongly between the two systems (~26% in the ASTRID and ~18% in the ZEPHYR of the total Pu in the core). The results reflect the optimization process trade-off between all isotopes to ensure better representativity. In light of these results a question arises - how would it be possible to achieve high representativity levels between different systems (material wise) when the uncertainties on the nuclear data are reduced dramatically?

Table 1. PSO results for the reference configuration search

Configuration	Matrix version	r_{RE}	PuO_2 content in MOX	Multiplication factor
Ref. at 20°C	COMAC-V01	0.988	29.35%	1.39777±0.00018
Ref. at 900°C	COMAC-V01	0.987	28.61%	1.37952±0.00018
Ref. at 900°C	UCOM-V01AB	0.964	31.48%	1.44828±0.00017

The second step, according to the presented methodology, is to identify the properties of the degraded configuration to ensure high representativity of the reactivity variation. Example of the optimization for the degraded core configuration is shown in Fig 6, where X and Y axes represent the PuO_2 content in the lower and upper degraded zones, respectively. The results show a similar behavior for all the examined temperatures; a zone with relatively low representativity values and high enrichment, a location where representativity is not feasible (representativity values equal to zero), and a region where the results are fulfilling the minimal criteria of 0.85. All the results for the single and multiple compacted zones representativity are summarized in detail in Table 2. The temperature impact for the two-zone configuration is mainly seen when the temperature rises from 20°C to 1000°C and above, where less fissile material is required to achieve the targeted value of the representativity. On the other hand, when a single zone is under investigation, the impact of the temperature is clearer, as can be seen in Table 2, when temperature rises and the required amount of PuO_2 is dropping for the same representativity level of 0.85.
The impact of the covariance matrix is examined as well for the reactivity variations for a single variation from 900°C to 1000°C. The results are shown in Table 3. In this case, as for the multiplication factor, the amount of PuO_2 required to reach the desired representativity increases when UCOM replaces COMAC in the optimization process. This is the direct result of the impact of the plutonium vector and the reduced uncertainties, similar to the multiplication factor optimization. A detailed description of this stage is published in [25].

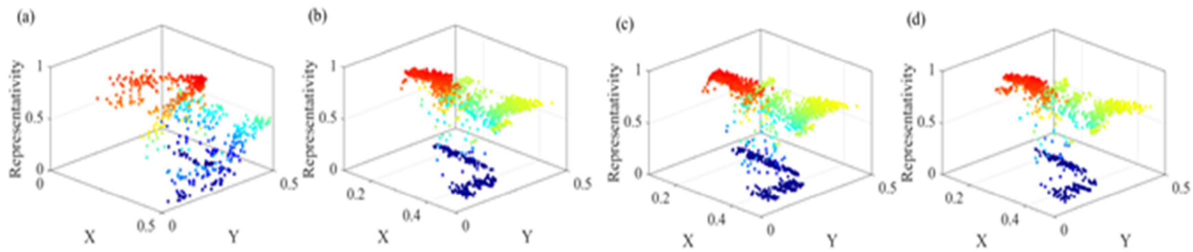


Fig 6. Results of the PSO for the reactivity variation representativity between reference configuration (Fig 4a) and two molten zones configurations (Fig 4c).
(a) 20°C. (b)1000°C. (c) 2000°C. (d) 3000°C.

Table 2. Approximate plutonium content of the ZEPHYR core using COMAC-V01AB

Configure/Temperature	PuO_2 Content		r_{RE} value
Configuration 1	Zone 1	Zone 2	
20°C	30%-35%	30%-35%	0.85-0.91
1000°C	20%-24%	20%-24%	0.85-0.87
2000°C	20%-24%	20%-24%	0.85-0.87
3000°C	20%-24%	20%-24%	0.85-0.87
Configuration 2			
20°C	28.3%	-	0.84
1000°C	22.5%	-	0.85
2000°C	22.3%	-	0.85
3000°C	22.2%	-	0.85

Table 3. Approximate plutonium content of the ZEPHYR core using UCOM-V01AB.

Configure/Temperature	PuO_2 Content		r_{RE} value
Configuration 1	Zone 1	Zone 2	
1000°C	22.5%-26.5%	22.5%-26.5%	0.85-0.91
Configuration 2			
1000°C	25.2%	-	0.85

5. Summary

This paper summarizes the continuous efforts that are being carried out by CEA Cadarache in the past three years in collaboration with Ben-Gurion University of the Negev, to examine the feasibility of representative severe accident of power reactor modelisation in zero-power facilities. This paper provides a selective overview of the project, including the methodology, the optimization considerations, and the physics underlying the trends in the results.
The main focus of the project is on the temperature effects, which play a major role in severe accident modeling with prominent impact on nuclear data. Therefore, in order to ensure high representation of the experimental system, those effects cannot be neglected and should be considered in the representativity process.
The proposed methodology is based on the optimization of the representativity factor (Eq. 1), with the utilization of Serpent MC, and is divided in two stages. The first stage is the optimization of a single fuel assembly, with the utilization of a PSO algorithm. The PSO allows an efficient search of the parameter space for relevant solutions. The relatively short time of the optimization calculation permits a wider search. The second stage of the project is the examination of the core level reactivity variation. In the case of the core optimization, the use of the PSO is not relevant, as it requires a large number of simulations in each iteration, which would result in an expensive simulation time. Therefore, and thanks to the relatively smooth gradients of the target function over the parameter search space, the Nelder-Mead simplex is selected as a faster method of optimization for this section.
The optimization results of the reactivity variation between two fuel assemblies are summarized in Fig 6 and Tables 2 and 3. The results show that for the different configurations and different temperatures it is possible to obtain a representative configuration, which ensures minimal value of 0.85.
The second optimization stage is currently under way. In this stage, it was found that the coupled core of the ZEPHYR reactor is not suitable for this kind of experimental program due to large differences between the reference and experimental systems. Preliminary optimization results indicate that it is possible to identify a highly representative configuration with “perfect fuel”. However, this requires further investigation (currently under way), and the impact of the utilization of the MASURCA fuel plates.
The presented methodology, based on the search for the most representative experimental configuration using state-of-the-art optimization algorithms is an innovative one. The utilization of highly representative configuration would provide indication for a large number of parameters (at this stage criticality and reactivity) of power systems in a controlled and safe environment of a zero-power reactor. The experimental data can then be used for neutronic code validation, nuclear data needs identification etc.

Acknowledgments

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