Integral Experiment Analyses in support to the OECD/NEA benchmarks on Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of SFRs (SFR-UAM)

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G. Rimpault, V. Huy

CEA, DEN, DER, SPRC, Cadarache, F-13108 St Paul-Lez-Durance, France
gerald.rimpault@cea.fr, virginie.huy@cea.fr

I. Kodeli

Institut Jožef Stefan, Jamova 39, 1000 Ljubljana, Slovenia
ivan.kodeli@ijs.si

ABSTRACT

Sodium fast reactors can answer three major challenges:
- Using the whole uranium ore (^{238}U and not only ^{235}U),
- Burning radioactive waste (Plutonium or minor actinides) in order to reduce the size of the ultimate storage,
- An enhanced safety.

Designing reactors with improved safety performance while preserving a sustainable source of energy at an economically competitive cost requires to improve the performance of the modelling tools. It is the purpose of the OECD/NEA sub-group on Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of Sodium-cooled Fast Reactors (SFR-UAM).

Two SFR cores are being studied: a large 3600 MWth oxide core and a medium 1000 MWth metallic core [1, 2]. For a reliable prediction of the characteristics of the core whose benchmark results are quite spread [3], it is necessary to use validated integral experiments of great confidence. It is the aim of the last task of the SFR-UAM task force [4, 5] to which this paper is contributing.

Some OECD experimental benchmarks [6, 7] (available from the ICSBEP and in the IRPhE experimental data bases) have been identified as relevant to the SFR-UAM core characteristics, with the use of sensitivities. These experiments have been analysed here with JEFF3.1.1 and provide a base

1.   Validation Exercises

The methods that were applied for the analysis of the specified theoretical exercises shall be used for the calculation of experiments. The calculated output quantities can be compared to the experimental values while considering the obtained uncertainties.

The validation experiments were chosen based on a similarity assessment between various experiments from the International Criticality Safety Benchmark Experiment

Handbook (ICSBEP) [6] and in the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE) [7] on one hand and the MET1000 and MOX3600 core assemblies, on the other hand [2].

2.   List of selected Experiments

The experiments used in this work are listed in Table 1 along with their fuel and structural material characteristics. The spectrum hardness indicator r is also given for mock-up reactors. This value r is the inverse of the difference between the average lethargy of neutrons disappearing through absorption or leakage $\overline{u_D}$ and the one of neutrons emmited by fission $\overline{u_P}$:

$$\frac{1}{r} = \overline{u_D} - \overline{u_P}$$

	Fuel	Fertile blanket or reflector	Diluant	r
FLATTOP [239]Pu	Pu-alloy (~4.8% [240]Pu)	Natural U reflector	-	-
JEZEBEL [239]Pu	Pu-alloy (4.5% [240]Pu) with 1.02 wt% Ga	-	-	-
JEZEBEL [240]Pu	Pu-alloy (20.1% [240]Pu) with 1.01 wt% Ga	-	-	-
ZPR-6/7	Inner core : U-Pu-Mo (Pu with 11% of Pu240) and UOx	Depleted U	Sodium and Iron	0.30
ZPR-6/7 High [240]Pu	Inner core : U-Pu-Mo (Pu with 27% of Pu240) and UOx	Depleted U	Sodium and Iron	0.32
SNEAK 7A	MOx 26.6% PuO2 (Pu with 8% [240]Pu)	Depleted U	Graphite	0.43
SNEAK 7B	MOx 26.6% PuO2 (Pu with 8% [240]Pu)	Depleted U	UOx with natural Uranium	0.45
MASURCA_ZONA2	MOx with 25 wt.% Pu (Pu with 18% [240]Pu)	Depleted U	Sodium and Steel	0.52

Table 1. Characteristics of the integral experiments critical masses used

One can note that this experimental database include international benchmarks from the IRPhE and ICSBEP database, as well as the experimental programmes performed in the CEA MASURCA facilities, not yet integrated in IRPhE.

The representability r_{RE} of an integral experiment E to a reactor concept R is a global indicator used to evaluate the similarity of the sensitivity profiles of two experiments. It is calculated (using the sensitivity of a target parameter, such as k_{eff}, to nuclear data S_E and S_R and a nuclear data covariance matrix D) by applying the following formula:

$$r_{RE} = \frac{S_R^T D S_E}{\sqrt{S_R^T D S_R} \sqrt{S_E^T D S_E}}$$

Sensitivities have been calculated with the ECCO/ERANOS code system [8] using JEFF3.1.1 nuclear data to which the COMAC-V1 matrix is associated for uncertainties [9]. Critical mass representability values of several Pu-fueled configurations to the SFR oxide core are given in Table 2.

Configuration	Representativity r_{RE}
ZPR-6/7	0.87
ZPR-6/7 High ^{240}Pu	0.90
SNEAK 7A	0.76
SNEAK 7B	0.84
MASURCA ZONA2	0.39

Table 2. Representability of the critical mass of Pu-fueled configurations to the SFR-UAM 3600 MWth oxide core critical mass. Values were calculated using COMAC-V1.

One has to note that representability calculations depend on the set of covariance matrices used. This indicator is thus particularly useful for transposition studies, for instance to foresee how an experiment could help reducing the uncertainty associated to a reactor concept.

Jezebel is a critical assembly made by the Los Alamos Scientific Laboratory in 1951. A total of three sub-assemblies was built: one made up of 95.5% at. of 239Pu (PUMET-FAST-001 according to the ICSBEP benchmark nomenclature), one consisting of 20.1% at.240Pu (PU-MET-FAST-002) and the last consisting of 98.0% at. 233U (U233-MET-FAST-001).This critical assembly has almost a spherical shape and is composed of four major pieces, of similar mass, for safety reasons. The critical masses from the ICSBEP database (FLATTOP ^{239}Pu, JEZEBEL ^{239}Pu and ^{240}Pu) are the only experiments that are likely to greatly affect nuclear data only in the high energies range, above 1-2MeV.

For ^{238}U inelastic and capture cross section, we benefit from a great number of experiments of Plutonium-fueled critical masses that are highly sensitive to this cross section,. Moreover, the simultaneous use of JEZEBEL and FLATTOP ^{239}Pu is particularly interesting to get access to ^{238}U inelastic cross sections. Indeed, JEZEBEL is a bare ^{239}Pu sphere and FLATTOP ^{239}Pu is similar to JEZEBEL (both in its geometry and its Plutonium content) except that it is surrounded by a natural Uranium .

Also, it seems important to use integral data sensitive to different isotopes (graphite, ^{56}Fe, ^{23}Na, ^{16}O, etc.) present in structural material. Indeed, this allows having access to different neutron flux spectra (and thus sensitivity profiles). For instance, ^{23}Na elastic scattering resonance at 2.85 keV causes a flux depression. This motivates the use of experiments which do not include ^{23}Na such as SNEAK7A/7B. Moreover, one has to keep in mind that eventual bias in structural material isotopes evaluations could induce large C/E for some experiments.

ZPR-6 Assembly 7 is a fast reactor core with mixed (Pu,U)-oxide fuel and sodium with a thick depleted-uranium reflector. A description of this experiment including the detailed specifications is given in the International Handbook of Evaluated Reactor Physics Benchmark Experiments under the acronym ZPR-LMFR-EXP-001. A variant of this assembly exhibits a central zone with a high Pu240 content.

The MASURCA ZONA2 core is part of an extensive experimental programme called BERENICE (Beta Effective Reactor Experiment for a New International Collaborative Evaluation) whose main objective was the measure of the effective fraction of delayed neutrons (βeff) by various methods. The programme is currently being evaluated in the IRPHE data base. Fuel pins are made of mixed oxide (U , Pu) O2 with a Pu / (U + Pu) content from about 25 to 27% , clad steel . The cross section of a fuel sub-assembly consists of a checkerboard of 16 fuel cells 2x2 pins , for a total 32 strips (U , Pu) O2 and sodium strips 32 (see Figure 15) . The

mostly used pins are the so-called " PIT " (Pu 18% 240Pu/Pu) pins and at the core periphery, a small amount of so-called " POA " (8% Pu 240Pu/Pu) pins are being used.

3.   C/E results on critical masses

Critical masses have been calculated with TRIPOLI4 [10] with the JEFF3.1.1 library. The JEFF3.1.1 library includes Probability Tables for a proper self-shielding of resonances in the Unresolved Resonance Region (URR). The geometry used is an as-built geometry hence without modelling approximations. Such calculations can be considered as benchmark values and incorporate no method approximation nor geometrical modelling errors.

C/E ratios as presented in Table 3 show values larger than one. It means that JEFF3.1.1 calculations are far bigger that measurement, however at less than 2 σ.

	C/E with TRIPOLI4 and JEFF3.1.1	Exp unc.	Nuclear data unc.	C/E-1²/Total unc ²	C/E-1²/Exp unc ²
FLATTOP_Pu239_keff	1.00396	0.00300	1.30E-02	9.32E-02	1.74E+00
JEZEBEL_Pu239_keff	1.00009	0.00250	1.24E-02	5.28E-05	1.30E-03
JEZEBEL_Pu240_keff	1.00433	0.00200	1.36E-02	1.01E-01	4.69E+00
SNEAK_7A_keff	1.00445	0.00400	1.30E-02	1.17E-01	1.24E+00
SNEAK_7B_keff	1.00140	0.00350	1.66E-02	7.10E-03	1.60E-01
MASURCA_ZONA2_keff	1.00447	0.00090	1.25E-02	1.29E-01	2.47E+01
ZPR6_7_keff	1.00196	0.00230	0.01514	1.68E-02	7.26E-01
ZPR6_7_High_Pu240_keff	0.99993	0.00220	1.48E-02	2.22E-05	1.01E-03

Table 3. C/E values for critical masses considered using JEFF3.1.1

The nuclear data uncertainties lie in the 1200-1660 pcm range which is far bigger than the experimental uncertainties. There is a possibility of improving nuclear data through an integral assimilation technique and hence the possibility to reduce the final SFR-UAM core characteristics uncertainty.

4. β_{eff} experimental validation

There are a number of available experiments for assessing the calculation of β_{eff} in the ICSBEP and in the IRPhEP experimental databases among which are JEZEBEL, SNEAK7A and SNEAK 7B. To these experiments, one can add the BERENICE experiments performed in MASURCA [5]. The importance of a neutron is needed for calculating β_{eff}, for which, the Iterated Fission Probability method (IFP) [11] is the most accurate method to obtain it with Monte Carlo, and has been implemented in various codes quite recently. Based on the interpretation calculations of α_{Rossi} and β_{eff} measurements, a series of calculation versus experiment comparisons is being done with modern tools such as MCNP, TRIPOLI4, SUSD3D, SERPENT and the latest evaluated nuclear data ENDF/B-VII.1, JEFF3.2, JENDL4.0. Uncertainty assessments due to nuclear data (including those for delayed neutron constant values) have been done using the SUSD3D and ERANOS tools. Uncertainties on delayed neutron constant values are only available in the JENDL4.0 library.

The calculations of uncertainties were carried out by JSI, CEA and, GRS for a series of experimental benchmarks: SNEAK 7A, SNEAK 7B, JEZEBEL, POPSY, BERENICE ZONA2, and, the SFR 3600MWth. These calculations of uncertainties have been done with various sets of covariance matrices including JENDL4.0 on which one can compare the calculations done at JSI, CEA and at GRS.

Benchmark experiment	Exp.	SUSD3D	PARTISN k-ratio	MCNP5 k-ratio	ERANOS	TRIPOLI IFP	MCNP6.1 IFP	SERPENT IFP
		ENDF7.0/-7.1*			JEFF3.2	ENDF7.1 /JEF3.2	ENDF7.1 /JEFF3.2	ENDF7.0 /JEFF31
Jezebel	194 ±10	185	186	186				187±1 /188±1
Skidoo	290 ±10	296	297					295±1 /294±1
Popsy	276 ±7	277	278	284				277±2 /287±2
Flat-top 23	360 ±9	374	375					374±2 /381±2
SNEAK-7A	395 ± 20	373	379	369	383	370 ± 3/ 391± 3	363 ± 3/ 391± 8	371±2 /385±2
SNEAK-7B	429 ± 22	419	429	415	426	417 ± 3/ 441± 3	427 ± 8/ 425 ± 8	417±2 /433±2
SNEAK-9C2	426 ± 19				384			383±2 /398±2
ZONA2	346 ± 11	344	351		362	335 ± 1/ 350 ± 1		
BFS-61	371 ± 60				383	370 ± 3/ 391± 3	363 ± 3/ 391± 8	
FCA-XIX-2	364 ± 9							368±2 /383±2
FCA-XIX-3	251 ± 4							250±1 /256±1

* ENDF7.1 stands for ENDF/B-VII.1

Table 4. Comparison of β_{eff} computational results with experiments

The use of Monte-Carlo code TRIPOLI4® [10] and its recent development of the Iterated Fission Probability method [11] allow us to improve the C/E ratio for calculating β_{eff}. The detailed representation of cores and the use of an energy dependency of the delayed neutron emission to the incident neutron energy are the major contributions to this improvement. Also, the improvement comes from the calculated terms used to derive β_{eff} from raw experimental measurements. The C/E ratios are greatly improved when using the reliable Noise measurement technique with 1.2% ± 3.2% for the ZONA2 core.

The uncertainty quantification process has been done using the deterministic code ERANOS, with the sensitivity analysis and uncertainty propagation leading to a 2.8% uncertainty for the ZONA2 cores whose main contributors are the delayed neutron fission yield and the fission cross section of ^{238}U.

Since uncertainties for delayed neutron constant values are available only in the JENDL4.0 library, a series of actions (differential measurements, models) are studied at CEA, ILL and Subatech-Nantes in order to provide in the future, new recommended values. The construction of the covariance matrices of the delayed fission yields of the ^{235}U, ^{238}U and ^{239}Pu

isotopes, including the correlations among these isotopes, is also underway in the scope of the cooperation between JSI and ENSIIE [12].

5.   Doppler measurements

Doppler coefficient is an important dynamic characteristic of the core. A review of relevant experiments in the IRPhEP database has identified a lack of experiments on Doppler. The SEFOR reactor has been built for the purpose of measuring the Doppler coefficient [13]. SEFOR documentation is not in the IRPhEP standard but has been used in the past [14] and is worth being investigated. Computational uncertainties in Doppler coefficient lie in the 100eV-100keV energy domain as illustrated by Figure 1 and are mainly due to the uncertainty in the flux level at the bottom edge of the fast reactor flux.

Figure 3. Doppler Effect (Nominal Temperature -> Fuel Melting Temperature) of an oxide SFR
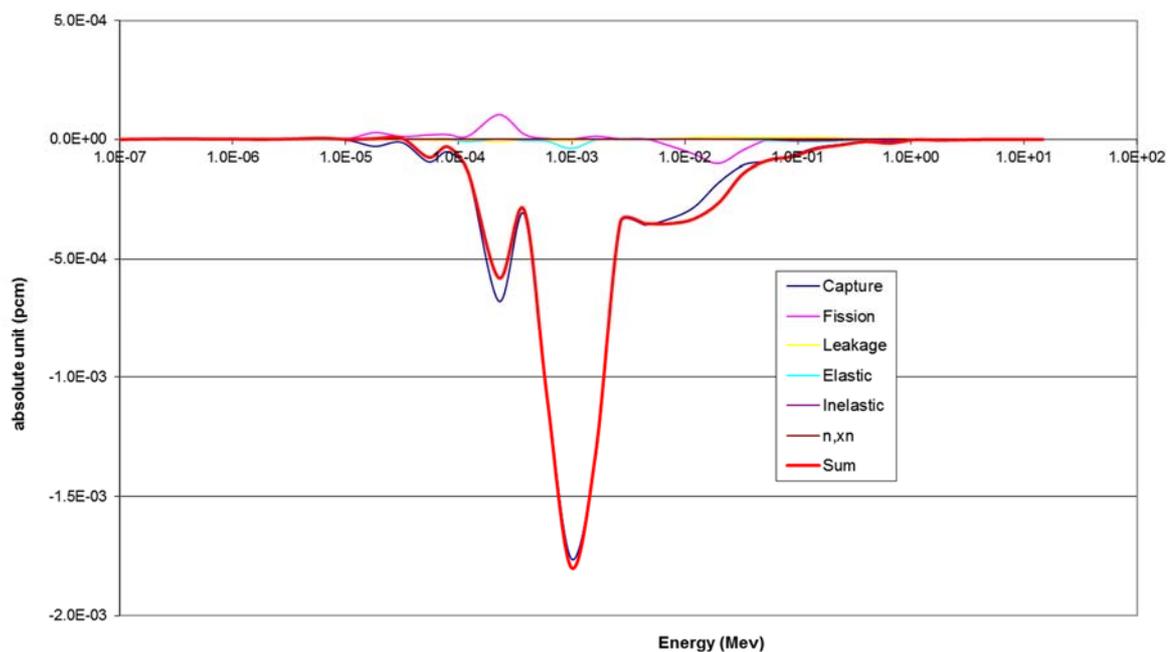
The SEFOR static tests were performed at power levels up to 20 MW while maintaining the average core coolant temperature constant at 678K. The reactivity effects due to power changes were measured by the reflector positions, adjusted to compensate the reactivity feedback. The Doppler coefficients were then evaluated by subtracting the contributions from the fuel axial expansion. Since SEFOR was particularly designed, using segmented fuel rods and dished fuel pellets, the reactivity change due to the axial expansion is as small as 5% of the total feedback, and its uncertainty has little affect on the Doppler reactivity evaluation.

Hence, the SEFOR static tests are recommended as an experimental validation of the Doppler calculations.

Careful attention should be given to the different sources of experimental uncertainties (fuel thermal conductivity, temperature increase, etc…). The resulting Doppler constants divided by β_{eff} (Tdρ/dT/βeff) for Core I and II are -2.61$ and -2.03$, respectively, according to the new analysis from Hazama & Tommasi [14]. The experimental uncertainty is reduced to 7%.

In the standard 2D cell representation, the heterogeneity of the B4C pin absorbers (12 in SEFOR l, 5 in SEFOR 2) must be taken into account. A calculation using the ECCO code is performed in which the B4C rod is surrounded by a corresponding part of the reactor and compared with an equivalent **homogeneous calculation.**

In Table 1, we present the values calculated using three different **approximations, a homogeneous cell model, a 2D heterogeneous model in which the boron pins are represented as an outer annular region and the third case in which a correction is made for the treatment of the boron pins.**

Modelling	SEFOR 1	SEFOR 2
D_{hom}	-810	-626
D_{het}	-871	-686
$D_{het} + \Delta D_{B4C}$	-893	-698

Table 5. SEFOR 1 & 2 modelling with ECCO/ERANOS

The C/E comparisons are presented for the two experiments with the corrected experimental values by [14] and the calculations using ECCO/ERANOS with a 2D heterogeneous model in which a correction is made for the treatment of the boron pins..

Core	C/E with JEF2.2	C/E with JEFF3.1
SEFOR 1	1.01	1.01
SEFOR 2	1.01	1.00

Table 6. SEFOR 1 & 2 C/E with ECCO/ERANOS

C/E values are within a ± 7 % range of uncertainties.

6.   Conclusions

The design of a SFR core implies the development and validation of scientific calculation tools. Notably, the use of neutronic codes aims at defining the characteristics of reactor cores with well-mastered accuracies. Nuclear data, the input parameters of these codes, constitute the main source of uncertainty in neutronic calculations.

The re-analysis of several experimental programmes in support to the SFR-UAM core benchmarks has been done in this paper. Reducing the bias on critical masses C/E due to deterministic methods and modeling approximations are of major concern. Thus, critical mass calculations were performed using the Monte-Carlo code TRIPOLI-4 on "as-built" geometries.

A great number of critical masses from the ICSBEP database (JEZEBEL [239]Pu, JEZEBEL [240]Puand FLATTOP [239]Pu), the IRPhE database (ZPR 6/7 assemblies, SNEAK 7A and 7B…) and MASURCA experimental programmes (ZONA2 etc.) have also been used. They provide both complementary and redundant information on nuclear data with a great diversity of sensitivity profiles which cover the energy range of interest. Moreover, their experimental uncertainties are much smaller than current nuclear data uncertainties calculated using COMAC-V1, so they have the capability to greatly reduce nuclear data uncertainties when used in an integral data assimilation.

As a perspective, performing an integral data assimilation would be a contribution to the improvement of our knowledge on nuclear data of interest for the SFR-UAM cores. Depending on the more or less urgent need of the core designers, assimilation results can be used as there are for core design or be used as guidelines for new evaluations.

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