NUMERICAL COMPARISONS BETWEEN NEUTRONIC CHARACTERISTICS OF MUSE4 CONFIGURATIONS AND XADS-TYPE MODELS

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Abstract

The representativity of a specific MUSE4 configuration (M4SC2) is analysed, from the nuclear data viewpoint, with respect to current concepts of eXperimental Accelerator Driven Systems (XADSs) with gas (He), Na and Pb/Bi coolants. In this context, data sensitivity/uncertainty analyses based on first-order perturbation theory calculations have been performed using the deterministic code ERANOS (Version 2.0) in conjunction with its adjusted nuclear data library ERALIB-1, leading to the determination of suitable representativity factors.
It is found that M4SC2 is quite representative of the XADSs with He and Na. However, in the case of the Pb/Bi system, effects of significant uncertainties associated with the data for these two nuclides and their low content in M4SC2, are clearly highlighted, resulting in much lower representativity factors in this case and thus indicating the need for additional experiments.

Introduction

In the field of waste management incorporating a transmutation option, accelerator driven systems (ADSs) represent an important alternative to conventional reactors due to their higher safety level when minor actinides such as Np and Am are loaded into the core. It has accordingly become necessary to extend the validation domain of calculational methods for critical fast reactors to the analysis of source-driven subcritical configurations.

To reach this goal, an experimental program, MUSE, has been launched in the MASURCA facility at CEA-Cadarache (France). In particular, the MUSE4 phase consists of the coupling of a PuO_2/UO_2+Na core with an external neutron source of high intensity [1]. The coupling has been achieved by employing a specially constructed pulsed neutron generator (GENEPI), which produces monoenergetic neutrons either via a $D(d,n)He^3$ reaction (2.7MeV neutrons) or a $T(d,n)He^4$ reaction (14.1MeV neutrons). The measurements being undertaken in the MUSE4 program constitute an important experimental database to be used for validating the calculational methods and data employed in the analysis of ADSs, e.g. ERANOS and its associated data libraries.

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In this context, specific investigations have currently been conducted to assess, via data sensitivity/uncertainty analyses, the representativity between MUSE4 and emerging concepts of eXperimental Accelerator-Driven Systems (XADSs). For this purpose, simplified RZ models for MUSE4 and different current XADS designs with gas (He), Na and Pb/Bi coolants (XADS_He, XADS_Pb/Bi, XADS_Na) have been set up. The fuel considered throughout, for MUSE4 as well as for all the XADSs, is 23-25% enriched PuO_2/UO_2 MOX fuel of the type used for the second SUPERPHENIX core. For the analyses, the deterministic code system ERANOS (Version 2.0) has been used. The parameters studied are the multiplication factor k_{eff}, a spectral index, F_5/F_8, viz. the fission rate of U^{235} relative to that of U^{238} at the centre of the fuel region, and a spatial index, $F_{5,1}/F_{5,2}$, viz. the U^{235} fission rate at the interface between spallation module and core mid-plane relative to that at the centre of the fuel zone.

Deterministic calculational scheme

General description of ERANOS

ERANOS-2.0 is a deterministic code system consisting of a variety of dedicated modules. In the present analysis, we are using the cell code ECCO [2], the RZ transport-theory code BISTRO [3] and first-order perturbation theory modules [4] in conjunction with the adjusted nuclear data library ERALIB-1 [5]. The numerical approximations are P1 for the anisotropy of scattering and S8 for the angular discretisation of the flux being computed in 33 energy groups. BISTRO solves the Boltzmann equation by means of a standard finite difference method.

Representativity factors and general approach

Employing a recently applied methodology with ERANOS [4], representativity factors r_{RE} between MUSE4 and the three XADS configurations (with He, Na and Pb/Bi coolants) have been evaluated for integral parameters such as the multiplication factor k_{eff} and specific reaction rate ratios, on the basis of first-order perturbation theory. These factors quantifying the impact of nuclear data uncertainties on the prediction of I, the parameter of interest (which depends on cross sections P_1, …, P_N), are obtained as follows :

Sensitivity coefficients S_i for $I(P_1, \ldots, P_N)$ are computed according to Equation (1) :

$$S_i = \frac{\Delta I}{I} \Big/ \frac{\Delta P_i}{P_i} \qquad (1)$$

The relative uncertainty s_I of I is obtained by using a covariance matrix D as shown in Equation (2) :

$$s_I^2 = S^t D S \qquad (2)$$

It should be noticed that D is associated with a specific nuclear data library.

For the parameter I, the representativity factor r_{RE} between two systems, e.g. MUSE and a given XADS, is determined from Equation (3) [4], the covariance matrix being taken from the adjusted data library ERALIB-1 :

$$r_{RE} = \frac{S_{XADS}^t D_{ERALIB} S_{MUSE}}{\sqrt{(S_{XADS}^t D_{ERALIB} S_{XADS})(S_{MUSE}^t D_{ERALIB} S_{MUSE})}} \qquad (3)$$

The value of r_{RE} lies between 0.0 and 1.0. The closer r_{RE} is to 1.0, the more representative is MUSE of the XADS.

Representativity factors can also be used to quantify the uncertainty reduction possible for the prediction of I on the basis of suitable integral measurements. This occurs via Equation (4) :

$$s^{2}_{I,XADS\_reduced} = s^{2}_{I,XADS}\left(1-\frac{r^{2}_{RE}}{1+s^{2}_{I,\exp}/s^{2}_{I,MUSE}}\right) \qquad (4)$$

Thereby, the experimental uncertainty of the parameter I, i.e. as measured in MUSE ($s_{I,exp}$), also plays a significant role. The smaller the experimental uncertainty, the stronger is the uncertainty reduction for the predicted value of I in the system of interest, the closeness of r_{RE} to 1.0 remaining an important aspect. In the most optimistic case (zero experimental uncertainty), Equation (4) becomes :

$$s^{2}_{I,XADS\_reduced} = s^{2}_{I,XADS}\left(1-r^{2}_{RE}\right) \qquad (5)$$

In the current study, the representativity between MUSE4 experiments and the different XADSs is evaluated based on the following scheme :

1. Assessment of nuclide-specific "integral sensitivities" on the basis of calculations of sensitivity coefficients S_i (see Equation (1)).
   The integral sensitivity to a given nuclide is the uncertainty of I obtained by assuming that (a) there is no correlation between data for different nuclides, (b) the individual reaction cross sections for the nuclide considered are also not correlated, and (c) the relative uncertainty for each of the nuclide cross sections is 100% over the whole energy range (< 20MeV). Effectively, an integral sensitivity is calculated on the basis of Equation (2) while assuming that the Matrix D is unity.
2. Determination of the uncertainty of I with the correct covariance matrix D from ERALIB-1 (see Equation (2)).
3. Calculation of the representativity factor r_{RE} (see Equation (3)).
4. Determination of the reduced uncertainty (see Equations (4) and (5)).

The reason for currently using the adjusted data library ERALIB-1 is to avoid the well known dominating effect of Pu^{239}, which was observed in the analysis of MUSE3 in conjunction with the (unadjusted) JEF-2.2 library [4]. However, the resulting uncertainties may be somewhat too small for the ADS situation, since the ERALIB adjustments were made solely on the basis of critical experiments. It is also necessary to underline the fact that methods uncertainties, as also uncertainties due to the external-source differences between MUSE4 and the XADSs, are not accounted for in the current analysis. Complementary studies, including methods/data comparisons made in the framework of benchmark exercises, are certainly important in this context [6].

General description

Models

The simplified RZ models considered for the XADSs are based on current PDS-XADS designs [7]. These are described in Figure 1 and in Table 1, in which only the most important materials are indicated [8].

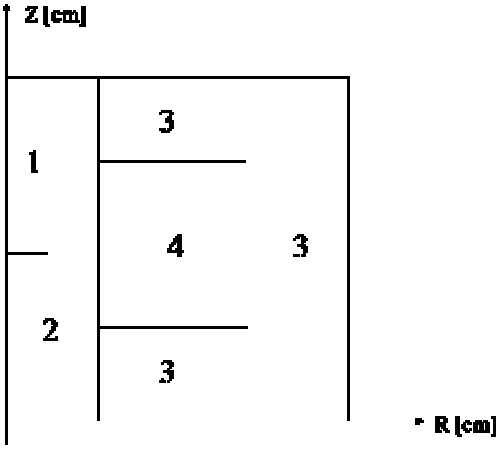

Fig. 1 : Definition of the homogenized zones for the three XADS models

Tab. 1 : Description of the homogenized zones of the three XADS models

Name	Zone 1	Zone 2	Zone 3	Zone 4
XADS_Pb/Bi	Void	Pb/Bi	Pb/Bi	PuO_2/UO_2 + Pb/Bi
XADS_He	Void	Pb/Bi	He + Steel	PuO_2/UO_2 + He
XADS_Na	Void	Pb/Bi	Na + Steel	PuO_2/UO_2 + Na

The basic principles to obtain the models were : (1) The volume of the spallation source (void + Pb/Bi) and the volume of the fuel region (Zone 4) correspond to the PDS-XADS design, (2) The outer radius of the reflector region (Zone 3) was adjusted to obtain a k_{eff}-value of 0.97.

The reference experimental set-up considered is the second subcritical configuration investigated in the MUSE4 program, viz. M4SC2 [8], the RZ model for which is described in Figure 2 and Table 2. For the sake of consistency with the XADSs, the original outer radius of Zone 4 has been modified slightly in order to achieve a k_{eff} value of 0.97.

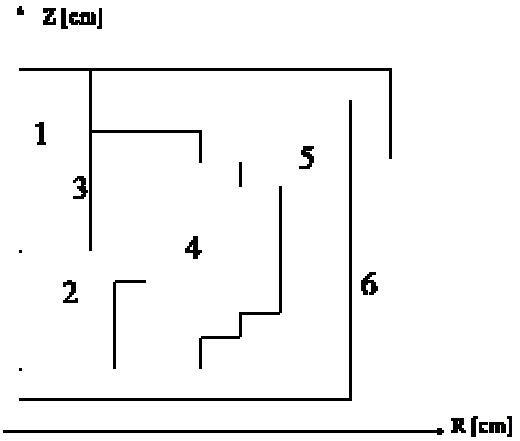

Fig. 2 : Definition of the homogenized zones for the M4SC2 model

Tab. 2 : Description of the homogenized zones of the M4SC2 model

Name	Zone 1	Zone 2	Zone 3	Zone 4	Zone 5	Zone 6
M4SC2	Void	Pb	Al	PuO_2/UO_2 + Na	Na + Steel	Steel

Parameters

As indicated earlier, representativity factors r_{RE} (see Equation (3)) between M4SC2 and XADS_He, XADS_Na and XADS_Pb/Bi are currently been considered for the three parameters listed below :

1. The multiplication factor k_{eff}.
2. F_5/F_8, viz. the fission of U^{235} relative to that U^{238} at the centre of the fuel region.
   This provides useful spectral information due to the different nature of U^{235} and U^{238} fission, the latter being a threshold reaction and the former not.
3. $F_{5,1}/F_{5,2}$, viz. the U^{235} fission rate at the interface between spallation module and core mid-plane relative to that at the centre of the fuel zone.
   This spatial index is sensitive to the geometry and composition of the spallation module.

Numerical results and interpretation

Representativity for the multiplication factor k_{eff}

Relative "integral sensitivities" are presented in Table 3. It is seen that the highest sensitivity, in each case, is to Pu^{239}. The contributions of the other nuclides are much smaller and quite similar in magnitude, except for Pb_{nat} and Bi^{209}, which have significant effects only in the XADS_Pb/Bi case.

Tab. 3 : Relative integral sensitivities (%) of k_{eff} with respect to the main isotopes

Isotopes	M4SC2	XADS_Na	XADS_Pb/Bi	XADS_He
U^{235}	0.8	1.9	1.7	1.8
U^{238}	3.1	2.6	3.7	0.4
Pu^{239}	83.0	84.6	78.3	85.5
Pu^{240}	4.8	4.6	4.7	6.2
Pu^{241}	1.6	4.6	4.1	4.4
Fe^{56}	3.2	0.3	1.3	0.2
Cr^{52}	1.4	0.5	0.1	0.7
Na^{23}	1.1	0.2	0.0	0.0
Pb_{nat}	0.0	0.1	2.8	0.1
Bi^{209}	0.0	0.1	3.0	0.1
Others	0.9	0.4	0.4	0.6

k_{eff}-uncertainties (again, only due to nuclear data uncertainties) are presented in Table 4, the main contributing nuclides being indicated in each case.

Tab. 4 : k_{eff}-uncertainties associated with the ERALIB-1 library

Name	Uncertainty on the k_{eff} (s_I)	Main contributors
M4SC2	± 162 pcm	Cr^{52}, Pu^{239}, Fe^{56} …
XADS_Na	± 163 pcm	Pu^{239}, Pu^{240}, Fe^{56} …
XADS_Pb/Bi	± 1021 pcm	Bi^{209}, Pb_{nat}, Pu^{239} …
XADS_He	± 199 pcm	Pu^{239}, Ni^{58}, Pu^{240} …

The uncertainties are similar for M4SC2, XADS_Na and XADS_He (s_I < 200 pcm), Pu^{239} being one of the main contributors in each configuration. Cr^{52}, a structural material isotope, is a major contributor for M4SC2, due to the larger quantity of this nuclide in the experimental set-up as compared to the XADSs. One also notes that the situation is completely different for the XADS_Pb/Bi case, where Pb_{nat} and Bi^{209} are the main contributors to the overall uncertainty (s_I > 1000 pcm), the data for these nuclides not having been adjusted in ERALIB-1.

The corresponding representativity factors are provided in Table 5. It is seen that, for k_{eff}, M4SC2 is quite representative of the XADS_Na and XADS_He, the corresponding r_{RE}-values being rather close to 1.0. On the contrary, the low presence of Pb_{nat} and the absence of Bi^{209} in M4SC2 lead to a low-valued representativity factor for the XADS_Pb/Bi. This indicates the need for additional integral measurements related to the data of lead and bismuth.

Tab. 5 : Representativity factors r_{RE} for k_{eff}

Compared systems	Representativity factor r_{RE}
M4SC2 ? XADS_Na	0.884
M4SC2 ? XADS_Pb/Bi	0.346
M4SC2 ? XADS_He	0.907

As indicated earlier, the degree to which the uncertainty of the prediction of a given parameter for an XADS can be reduced via an integral measurement depends on the corresponding representativity factor r_{RE} (see Equations (3) and (4)). Thereby, the experimental uncertainty associated with the measurement also plays a key role. Table 6 shows, as illustration, the k_{eff} uncertainty reduction for the case of the XADS_He assuming different values of the experimental uncertainty in M4SC2 [8].

Tab. 6 : Example of k_{eff} uncertainty reduction for the XADS_He system

For the k_{eff} prediction	Value (with ERALIB-1)
$s_{I,XADS}$: Uncertainty for XADS_He	± 199 pcm
$s_{I,MUSE}$: Uncertainty for M4SC2	± 162 pcm
r_{RE} : Representativity factor	0.907
$s_{I,XADS\_reduced}$: Reduced uncertainty for XADS_He (with an $s_{I,exp}$ experimental uncertainty of ± 0 pcm)	± 77 pcm
$s_{I,XADS\_reduced}$: Reduced uncertainty for XADS_He (with an $s_{I,exp}$ experimental uncertainty of ± 100 pcm)	± 127 pcm
$s_{I,XADS\_reduced}$: Reduced uncertainty for XADS_He (with an $s_{I,exp}$ experimental uncertainty of ± 200 pcm)	± 163 pcm

Once again, only uncertainties associated with nuclear data are being accounted for in the present analysis. Nevertheless, the sensitivity coefficients considered (see Equation (1)) in determining the corresponding representativity factors do permit obtaining important qualitative indications on the

correlation between the compared systems. In the following sections, related to the two other integral parameters under consideration, the aspect of uncertainty reduction is not treated explicitly, the different XADSs being compared with M4SC2 solely on the basis of integral sensitivities and representativity factors.

Representativity for F_5/F_8

The relative integral sensitivities to the main isotopes are given in Table 7 for the various cases. The contributions of U^{235} and U^{238}, these isotopes having a direct impact on the reaction rate ratio under consideration, are, as expected, larger than in the previous (k_{eff}) case. In addition, a significant contribution of Pu^{239} is still observed for all the systems, while Na^{23}, Pb_{nat} and Bi^{209} have significant effects only in the systems in which they are present in an important way.

Tab. 7 : Relative integral sensitivities (%) of the spectral ratio F_5/F_8 to the main isotopes

Isotopes	M4SC2	XADS_Na	XADS_Pb/Bi	XADS_He
U^{235}	37.3	33.6	32.8	38.6
U^{238}	33.1	33.1	33.0	35.4
Pu^{239}	13.3	11.7	10.7	11.7
Pu^{240}	0.8	1.3	1.2	1.2
Pu^{241}	0.2	0.5	0.5	0.5
Fe^{56}	6.3	7.2	5.4	8.4
Cr^{52}	2.0	0.9	0.5	1.6
Na^{23}	5.0	10.8	0.0	0.0
Pb_{nat}	0.4	0.1	6.8	0.2
Bi^{209}	0.0	0.1	8.5	0.2
Others	1.6	0.5	0.5	2.1

The corresponding representativity factors are given in Table 8. These are similar to the results for k_{eff}. The subcritical core of M4SC2 is representative of the XADS_Na and XADS_He. Again, the low representativity with respect to the XADS_Pb/Bi reflects deficiencies associated with the data for Pb_{nat} and Bi^{209}, as well as the low content of these nuclides in the experimental configuration.

Tab. 8 : Representativity factors r_{RE} for F_5/F_8

Compared systems	Representativity factor r_{RE}
M4SC2 ? XADS_Na	0.853
M4SC2 ? XADS_Pb/Bi	0.264
M4SC2 ? XADS_He	0.885

Representativity for $F_{5,1}/F_{5,2}$

Relative integral sensitivities for this spatial index are presented in Table 9. The contributions of the individual nuclides are significantly different from the previous two cases (see Table 3 and Table 7), indicating the significant impact of the spallation module on this particular parameter. The contributions of Pb_{nat} and Bi^{209} (except of course for M4SC2, in which Bi^{209} does not occur) are seen to increase quite markedly.

Tab. 9 : Relative integral sensitivities (%) to the main isotopes for $F_{5,1}/F_{5,2}$

Isotopes	M4SC2	XADS_Na	XADS_Pb/Bi	XADS_He
U^{235}	0.2	0.3	0.3	0.1
U^{238}	34.5	15.7	22.4	15.9
Pu^{239}	20.9	5.5	1.0	6.0
Pu^{240}	4.9	3.5	5.9	1.3
Fe^{56}	0.5	4.6	39.9	37.2
Fe^{57}	0.6	2.3	6.2	4.9
Cr^{52}	3.8	3.2	1.4	0.1
Ni^{58}	0.5	0.7	1.3	5.7
Na^{23}	16.8	23.2	0.0	0.0
Pb_{nat}	15.3	20.7	15.0	15.0
Bi^{209}	0.0	19.0	4.8	13.4
Others	1.8	1.3	1.9	0.3

As to be expected, the representativity factors being given in Table 10 are also significantly different from the corresponding values in the previous sections. Generally speaking, the r_{RE} factors are much smaller. This is due to the different source regions, which are quite dissimilar in terms of geometry and material composition, e.g. the source module of M4SC2, as mentioned above, has no Bi^{209}. Additional calculations for the three XADSs, carried out assuming modified targets in which Bi^{209} is replaced by Pb_{nat}, indeed yielded significantly larger representativity factors (also shown in Table 10).

Tab. 10 : Representativity factors r_{RE} for $F_{5,1}/F_{5,2}$

Compared systems	Representativity factor r_{RE}	Representativity factor r_{RE} (no Bi^{209} in XADS spallation module)
M4SC2 ? XADS_Na	0.258	0.552
M4SC2 ? XADS_Pb/Bi	0.066	0.383
M4SC2 ? XADS_He	0.259	0.556

Conclusions

Investigations related to k_{eff} and reaction rate ratios have been conducted to assess the representativity between MUSE4 and various concepts of eXperimental Accelerator-Driven Systems (XADSs). In this context, sensitivity/uncertainty calculations have been performed using the deterministic code system ERANOS (Version 2.0) in conjunction with its adjusted data library ERALIB-1 based on the JEF-2.2 evaluation. Employing a recently applied methodology [4], representativity factors r_{RE} between the second subcritical MUSE4 core (M4SC2) and the three current PDS-XADS designs (with He, Na and Pb/Bi coolants) have been evaluated for different integral parameters.

Specifically, it has been found that the representativity between M4SC2 and an XADS with Na or He coolants is, in general, quite satisfactory, except for the region with the source module. In the case of an XADS with Pb/Bi coolant, the relatively low representativity results from the large uncertainties

associated with the nuclear data for Pb_{nat} and Bi^{209}, as also the low content of these nuclides in the experimental configuration. This clearly indicates a need for additional integral experiments.

It is necessary to underline the fact that only data uncertainties have been accounted for in the present study. Methods uncertainties and combined methods/data effects have not been considered, nor have the effects of differences in the external neutron source [9]. Further investigations are called for in this context, e.g. detailed comparisons in the framework of specific benchmark exercises [6].

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