Neutronic benchmark on the 2400 MW gas-cooled fast reactor design

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Abstract

The 2400 MWth Gas-Cooled Fast Reactor (GCFR), with plate-type carbide/SiC CERCER fuel, is an innovative design exhibiting many attractive features among which sustainability achieved with an internal breeding gain close to zero and feedback coefficients enabling an excellent behavior under some safety transients. This paper summarizes the analytical results of an international benchmark exercise being set up within the European Union to verify the neutronic tools and associated nuclear data libraries currently used for helping in finalizing the design of the GCFR within the European Union. A rather simple homogenized 2D model has been specified for the first phase of this benchmark. The computational tools being used in the analysis include both a stochastic and a deterministic code, MCNP and ERANOS, respectively, with nuclear data essentially based on the JEF-2.2 data library. The overall results indicate that the agreement of the solutions provided by the different participants is satisfactory. The most significant discrepancy, which can be partly attributed to different ERANOS options, is observed in the case of the end of life reactivity and amounts to a few dollars. The rather positive outcome of this initial phase of the benchmark has allowed identifying deficiencies in the analytical tools and serves as a basis for the definition of subsequent phases. It might also help to identify potential ways to improve the design.

KEYWORDS: GCFR, Neutronics, Benchmark, Reactivity coefficients, OCTOPUS, ERANOS

1. Introduction

Within the European Union, several calculational tools and nuclear data libraries are currently used in the framework of the research and development of Gas-Cooled Fast Reactor (GCFR) designs. In addition to stochastic tools, like MCNP, one of the most important deterministic program being employed is ERANOS, a code system which is currently used by various institutes and companies to finalize the GCFR pre-conceptual design. ERANOS and the associated nuclear data libraries were originally developed for liquid metal reactors. In the latest version [1], various improvements have been incorporated. These new features allow treating new type GCFR sub-assemblies characterized by special geometries and strong fuel heterogeneities. Since it is very important to verify them prior routinely use, CEA has set up,

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in collaboration with the European partners, a GCFR neutronic benchmark. The current reference design serving as a basis for the benchmark calculations is that of a large system (2400 MWth), which is an innovative concept based upon plate-type carbide/SiC CERCER fuel, helium coolant and SiC structural material. Whereas NRG uses the code coupling system OCTOPUS [2], in which the Monte Carlo code MCNP4C is coupled to the inventory code FISPACT, the other organizations involved in the analyses use ERANOS, the code being installed on local computers. The benchmark model, which is currently characterized by homogeneous sub-assemblies and regions, will be progressively refined.

2. Benchmark definition and participants

2.1 Benchmark definition

We recall that the 2D model has been derived based on the main characteristics of a typical GCFR core (see Tab. 1).

Table 1: Main characteristics of the 2400 MWth GCFR core

CERCER Fuel	(U,Pu)C 56% vol – (SiC Matrix 16%vol. + He gaps 28%vol.)
Average Pvol (MW/m^3)	100
Reactor Power (MWt/MWe)	2400/1158
Volume (m^3)	24
Diameter (m) / Height (m)	4.44/1.55
H/D	0.35
SiC structures (%vol.)	20
Gas (%vol.)	51.2
[He coolant / He gaps]	[40.1 / 11.1]
(U,Pu)C (%vol.)	22.4
SiC matrix (%vol.)	6.4
ΔP (bar)	-0.62
He pressure (bar)	70
T_{max} cladding BOL (°C)	1075
T_{max} fuel BOL (°C)	1210
TRU content (%)	15.2
TRU inventory (tons)	54.4
Pu inventory (tons/GWe)	7.7
Core management	3×831 = 2493 EFPD
Average burnup (FIMA)	~ 10 %

In this model, the envisaged core region (15% Pu in the fuel) is subdivided into two radial zones (inner and outer core with slightly different Pu contents) and eight axial layers; the reflector/shield region consists of 3 zones (top, bottom and radial reflector/shields). The individual fuel and reflector/shield sub-assemblies are all homogeneous. Within each region, the temperature distribution is space- and time-independent, amounting to 990°C and 665°C, in the core and reflector/shield, respectively. The full cycle length amounts to 2493

Equivalent Full Power Days (EFPD), simulating a 3-batch loading pattern of 831 days each.

The following integral parameters were to be calculated for initial (BOL) and fully burnt (EOL) core conditions:

1. Reactivity.
2. Core Doppler effect, expressed as reactivity difference between two core states (T_{fuel}=990°C and T_{fuel}=180°C), the core dimensions being obviously the same.
3. Core depressurization reactivity, i.e. the reactivity difference between nominal and fully depressurized core conditions (1 bar pressure).
4. Delayed neutron fraction (β_{eff}).
5. Total breeding gain [3].

The envisaged future phases of the benchmark are explicit 3D plate-type sub-assemblies in conjunction with the same 2-D core model, as well as more rigorous three-dimensional, Hex-Z core models in conjunction with homogeneous sub-assemblies.

2.2 Participants

Tab. 2 displays the list of the participating organizations. Also provided is summary information on the specific code and data library, including the main input options. Obviously, the transport-theory approximation required by discrete-ordinates methods has been left out in the case of the NRG analyses.

Table 2: Participants and main simulation options. FP- fission products; BU – burnup.

	CEA	***NEXIA***	***PSI (ERALIB1)***	***PSI (JECCOLIB2)***	***NRG-std***	***NRG-fine***
Code	ERANOS				OCTOPUS	
Library	ERALIB1			JEF-2.2		
FP	6 lumped-FP	87FP	6 lumped- FP		77FP	
Transport option	$P_0 S_4$	$P_1 S_8$			---	---
Radial BU meshes	2		10		2	5
BU steps	3		9		3	90

The methods involved will be described in the next section.

3. Computational methods and nuclear data

3.1 OCTOPUS code system

NRG uses OCTOPUS [2,4], a modular system, in which various spectrum and burn-up codes can be linked together on the basis of binary interface files. The structure of this code system is flexible enough to allow the coupling of other type of codes as well, like uncertainty analysis codes, or codes for generation of nuclear databases required for full core reactor simulation. Specifically, the stochastic spectrum code MCNP4C3 [5-6] has been used in combination with the burn-up inventory code FISPACT [7]. JEF-2.2 data was employed, except for two nuclides (^{244}Am and ^{244}Cm), for which data was used from JENDL-3.2 and ENDF/B-VI.5, respectively.

The 3-D flux distribution is calculated for each burnup step using MCNP, and in a separate OCTOPUS module the cross sections for each active isotope (taken from the MCNP point

cross-section library) are collapsed to self-shielded few-group cross sections in 172 groups, using the spectrum in each burnup zone. A separate FISPACT run computes for each burnup zone the new isotopic composition using these few-group cross sections. The flux to be used by FISPACT is calculated before each burnup step from the total reactor power, the isotopic composition of each burnup zone, the flux distribution, and the energy released per fission and capture for each nuclide. The flux and reaction rate tallies produced by MCNP are also normalized using the same normalization factor. The self-shielded flux in 172 groups is used in FISPACT to collapse the cross section data for those nuclides that are not available in the MCNP library. These are nuclides which are not being explicitly considered in the MCNP runs, and for which no self-shielding is taken into account.

3.2 ERANOS code system

ERANOS [1] is a deterministic code system which was originally developed for the simulation of sodium-cooled fast reactors. In its current version (ERANOS-2.0), dedicated features have been added, which are particularly suited to analyze gas-cooled fast reactors as well as accelerator driven systems. Except NRG, all participants have used ERANOS-2.0 in the analysis of the benchmark exercise. Some of them required in-house adaptations, which will be discussed later in this section.

The modular structure of ERANOS enables the user to link the individual programs in different ways, depending on the type of application. Important modules are e.g. ECCO, TGV/VARIANT (not used in the current analysis) and BISTRO. ECCO is a lattice code, which can be used in conjunction with a variety of arrangements including (1) 2-D rectangular lattices of cylindrical and/or square pins, (2) 3-D slab geometry, and (3) 2-D hexagonal lattices of cylindrical pins. It is based on the collision probability method to generate broad-group cross sections, the subgroup method being additionally used to treat resonance self-shielding effects. ECCO cross sections can subsequently be used in full core calculations performed either with the 3-D nodal variational transport code TGV/VARIANT or the finite difference code BISTRO which supports both S_N-transport- and diffusion-theory methods. BISTRO can handle 2-D (X-Y and R-Z) as well as 1-D (spherical, cylindrical and planar) geometries.

The ERANOS-2.0 package contains several JEF-2.2 based (unadjusted) data libraries (JECCOLIB2, referred to as J2 in the following tables) for different energy structures ranging from 1968 to 33 groups. The fine group library in 1968 groups includes cross-sections for 37 important nuclides needed in detailed slowing-down calculations. Correspondingly, ERALIB1 (referred to as E1 in the following tables) consists of adjusted cross-sections, which were derived from the unadjusted values based on a large number of integral measurements performed on critical fast-spectrum configurations.

3.2.1 PSI

At PSI, the required calculations were performed using ERALIB1 and JECCOLIB2. The required cell calculations were performed with ECCO for the various homogeneous zones of the benchmark model, allowing to generate self-shielded cross-sections in 33 neutron groups. Thereby, the so called "Reference Route" was used. This approach is based upon slowing-down calculations in 1968 fine groups, the fuel regions being computed in the fundamental mode spectrum, with the subgroup method being used to treat resonance self-shielding effects within each fine group. In the non-fuel regions, the slowing-down source being specifically used corresponded to the average spectrum of the fuel region.

The forward and adjoint flux calculations needed for computing the multiplication factor, k_{eff}, kinetic parameters, as well as reactivity effects, were carried out using the code BISTRO in conjunction with these 33 neutron broad group cross-sections and P_1S_8-approximations. In the fuel zones, viz. inner and outer core regions, 10 meshes were used in the radial direction, whereas the active core height was subdivided into 20 meshes of the same thickness; the zones with reflector material were modeled with 10 subdivisions in each direction. The agreement of k_{eff} observed between forward and corresponding adjoint calculation was always excellent within a few pcm (1 pcm = 10^{-5}), giving so far a certain confidence in this methodology. Only the solid fission products have been considered (the gaseous fission products are supposed not to be retained in the fuel).

In the burn-up calculations, available data for six solid pseudo fission products for the main actinides were used. The flux distribution in space and energy, and thus the one-group microscopic cross-sections of the fuel nuclides, were calculated at the beginning and at the end of 9 periods of 277 EFPDs, the core region being subdivided, for the purpose of condensation in energy, radially into 10 cylindrical rings and axially into 10 axial layers of equal thickness, in order to solve the (one-group) burn-up equations in these (100) regions. Thereby, the required microscopic cross sections in 33 groups were those for fresh fuel compositions, i.e. the self-shielding of the resonance cross-sections was not repeated in the different burn-up steps. At the end of shorter periods of ~23 EFPDs (there were 12 such periods of the same duration within one longer period of 277 EFPDs), the flux was renormalized to maintain the input thermal power, i.e. 2400 MW.

3.2.2 CEA

The ERANOS calculation scheme used at CEA for scoping studies has the following features:

- Cross sections generated by the ECCO module, using the ERALIB1 adjusted nuclear data library.
- For the homogeneous representation of the reactor cells, fine-group ECCO cell calculations were performed using a fine-group structure (1968 groups) and the results were condensed in a 33 broad-group scheme.
- In a second step a cylindrical (R-Z) core model was used. The calculation of the neutronic flux and derived parameters were carried out with the BISTRO S_n module (S_4 option), using transport theory in a 33 broad-group scheme.

Because of the simplicity of the approach, some other calculations were performed in order to obtain a reference result (see parametric study below)

4. Analyses of benchmark results

4.1 Reactivity, reactivity coefficients and breeding gain

In this paragraph, the results are reviewed and analyzed.

4.1.1 Reactivity

The results along with the computational tools (see also Table 2) are displayed in Tab. 3.

In this table, and throughout the paper, the OCTOPUS results include the 1σ standard deviation. At BOL, the discrepancy of the calculated reactivity is rather modest (maximum deviation of +164/-124 pcm, with respect to a mean value of 2758 pcm). The EOL-values, on the contrary, show a much larger dispersion of +473/-489 pcm, with respect to a mean value of -1361 pcm.

Table 3: Results for the reactivity (BOL and EOL) by participant

	CEA	*NEXIA*	*PSI (E1)*	*PSI (J2)*	*NRG std.*	*NRG fine*
Code	ERANOS				OCTOPUS	
Library	E1			JEF-2.2		
Fission products	6 lumped FP	87 FP	6 lumped FP		77 FP	
Transport option	$P_0 S_4$	$P_1 S_8$			-	
Radial BU meshes	2		10		2	5
BU steps	3		20		3	90
Reactivity BOL (pcm)	**2922**	**2719**	**2875**	**2670**	**2727 ± 63**	**2634 ± 38**
Reactivity EOL (pcm)	**-1850**	**-1372**	**-1348**	**-1182**	**-1529 ± 63**	**-888 ± 44**

Parametric study

In order to explain these differences, a parametric study has been launched. Starting point is the set of options employed in the CEA calculation. The following ERANOS input features have been closely investigated:

1. Nuclear data library: An additional calculation has been made, which uses unadjusted (J2) instead of adjusted data (E1).
2. Use of lumped fission products: The design scheme uses 6 lumped fission products. These pseudo cross-sections are aimed at simulating the absorption of the individual fission products in Na-cooled fast reactors, which originate mostly from ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu. A more precise burn-up calculation has been performed based upon the use of 87 explicit fission products.
3. Number of radial BU meshes: An additional burn-up calculation has been carried out based on the use of 5 (instead of 2) radial meshes. The finer discretization in the radial direction was used for the purpose of solving the burn-up equations on a finer spatial grid. The cross-sections and meshing used in the transport-theory calculations remained the same.
4. Number and size of the burn-up steps: A refined calculation has been made using 90 time steps of maximum 30 EFPD, the step size being significantly smaller during the first 30 EFPD. The flux calculation was repeated at the beginning of each step.
5. Transport-theory option: A more precise P_1S_8 approximation was used (instead of P_0S_4) for the treatment of the scattering anisotropy and the angular development of the flux, respectively.

The results are summarized in Tab. 4. At this point, it is important noticing that the 6 lumped fission products used by CEA and PSI in their original calculations (see Tab. 3) were different, which is the main cause for the different EOL reactivities obtained by these two institutions. The CEA calculational scheme used solid and gaseous fission products, implying that all fission products are kept in the plate-type sub-assembly. On the contrary, the standard option for pin-type-fuel fast reactors was used in the PSI calculations, implying that just the solid fission products are kept in the fuel, whereas the volatile gaseous fission products do escape. Adding the lumped gaseous fission products in the PSI calculation is found to result

in a 800 pcm reactivity decrease at EOL.

Table 4: Reactivity and reactivity variations ($\Delta\rho$) due to the use of different ERANOS options. The values in the second column from the left are CEA results (see Table 3).

Influence of the nuclear data library			**$\Delta\rho$ (pcm)**
	E1	*J2*	
BOL	2922	2721	**-201**
EOL	-1850	-1683	**+167**
Influence of the FP cross-sections			
	6 lumped FP's	*88 explicit FP*	
EOL	-1850	-1017	**+833**
Influence of the number of radial BU meshes			
	2 meshes	*5 meshes*	
EOL	-1850	-1997	**-147**
Influence of the number of BU steps			
	3 steps	*90 steps*	
EOL	-1850	-1887	**-37**
Influence of the transport-theory options			
	$P_0 S_4$	$P_1 S_8$	
BOL	2922	2868	**-54**
EOL	-1850	-1903	**-54**

Summary of results for reactivity

Based upon the results of the previous parametric study (see Tab. 4), the reactivities (see Tab. 3) have been extrapolated to hypothetical values which would result from the use of a more consistent set of approximations among the different participants. The new results are summarized in Tab. 5.

Table 5: Benchmark results before and after introducing corrections for differences in methods/data

	CEA	***NEXIA***	***PSI (J2)***	***NRG fine***
Reactivity BOL	*2922*	*2719*	*2670*	*2634 ± 38*
Library(JEF2.2)	-201	-201	-	-
Transport option(P_1, S_8)	-54	-	-	-
Reactivity BOL	**2667**	**2518**	**2670**	**2634 ± 38**
Reactivity EOL	*-1850*	*-1372*	*-1182*	*-888 ± 44*
Library (JEF2.2)	+167	+167	-	-
Fission products (explicit)	+833	-	+833	-
Radial core meshes (5)	-147	-147	+53	-
BU steps (90)	-37	-37	-37	-
Transport option (P_1, S_8)	-54	-	-	-
Solid+Gaseous FP	-	-	-800	-
Reactivity EOL	**-1088**	**-1389**	**-1133**	**-888 ± 44**

The correction of +53 pcm ("Radial core meshes (5)") for the PSI value (instead of -147 pcm for the CEA and NEXIA values) is the result of an additional investigation: In the PSI calculation, the EOL reactivity would namely increase by 200 pcm when using exactly the

same discretization scheme in both directions (10 radial and axial meshes), i.e. with respect to burnup meshing employed in the CEA calculation.

4.1.2 Reactivity coefficients and total breeding gain

The discrepancies being observed for these parameters are rather small. Nevertheless, the methods/data influence was studied in a similar manner as for the reactivity, showing that this effect is marginal. The final extrapolated values for the reactivity coefficients, delayed neutron fraction and breeding gain are summarized in Tab. 6.

Table 6: Reactivity coefficients, delayed neutron fraction and total breeding gain (TBG)

		CEA	*NEXIA*	*PSI (J2)*	*NRG fine*
Doppler effect (pcm)	**BOL**	1909	1934	1916	1845 ± 59
	EOL	1247	-	1296	1126 ± 59
Coolant depressurization reactivity (pcm)	**BOL**	213	186	214	249 ± 17
	EOL	271	274	263	287 ± 16
β_{eff} (pcm)	**BOL**	392	401	389	391 ± 9
	EOL	350	-	356	352 ± 8
TBG (pcm)	**BOL**	-1.51	-1.49	-	-1.47
	EOL	-0.04	-0.01	-0.02	-0.02

4.2 Sensitivity/uncertainty analysis to nuclear data

An analysis of the sensitivity and uncertainty on the benchmark results to the nuclear data has been performed using ERANOS, and on the basis of the PSI results. Use was made of "Extended Generalized Perturbation Theory" (EGPT) by means of dedicated procedures available in ERANOS-2.0, to compute the required sensitivity coefficients for k_{eff}. Reactivity variations, including core Doppler effect and coolant void depressurization, were analyzed in a similar manner. The resulting agreement of all these parameters computed with and without perturbation theory was excellent within a few ‰.

The uncertainty of these parameters due to nuclear data uncertainties was assessed in conjunction with these sensitivity coefficients, based upon the additional use of covariance matrices in 15 neutron groups available for the main actinides and structural materials.

Tab. 7 displays the results for BOL conditions.

Table7: Uncertainties (%, BOL conditions)

	PSI(E1)	*PSI(J2)*
k_{eff}	± 0.3	± 1.4
Doppler effect	± 1.5	± 3.7
Coolant depressurization reactivity	± 2.1	± 4.9

In the case of the adjusted library (ERALIB1), the following decomposition of the effect for the different parameters which have been investigated, is conveniently given in terms of cross sections for the individual nuclides:

1. **k_{eff}**: Fission of the different Pu-isotopes (0.1% each), capture and elastic scattering of Zr (0.1% each).

2. **Core Doppler effect**: Fission and capture of ^{239}Pu (0.9% each), elastic scattering of C (0.7%) and capture of ^{240}Pu (0.5%).
3. **Coolant depressurization reactivity**: Inelastic scattering of ^{238}U (1.3%), capture of ^{240}Pu and elastic scattering of C (0.7% each).

In the case of the unadjusted library (JECCOLIB2), the obviously larger uncertainties being observed are found to be largely dominated by the cross sections of ^{239}Pu.

5. Discussion

The discrepancies between calculations performed on the basis of 6 lumped fission products instead of 87 explicit fission products are very important (833 pcm in reactivity) and show that the lumped fission products currently available in the ERANOS libraries are not suitable for GCFR calculations. Therefore, new lumped fission products dedicated to GCFR cores need to be processed.

After suitable corrections of the original results, as summarized in Tab. 5, the average reactivity value amounts to (2622 ± 62) pcm at BOL, and to (-1124 ± 178) pcm at EOL. Thus, in comparison with the uncorrected results (see Tab. 3), the spread has been substantially reduced, particularly for EOL conditions, i.e. from initially 518 pcm (1σ) to 178 pcm (1σ). By considering only the ERANOS results, the average reactivity value for EOL conditions is (-1203 ± 132) pcm, and the dispersion (difference between the highest and the lowest reactivity value) is reduced from an intial 501 pcm to 301 pcm. Therefore, the spread of the EOL reactivity values can only partially be attributed to the different approach being used in the deterministic and Monte-Carlo calculations (e.g. point-wise versus group-wise cross-sections, different resonance treatment, approximations in the S_N transport method).

The importance of defining the reference options within ERANOS appears clearly when comparing initial results from the participants. Once important options are identified, corrected results are far less discrepant and the best estimate result can then be compared to the Monte-Carlo result in a satisfactory manner.

The uncertainty analysis with respect to nuclear data uncertainties shows that the resulting uncertainties in reactivity (~290 pcm in the case of ERALIB1 and ~1360 pcm for JECCOLIB2) in fact overshadow the spread of the results provided by the participants. The covariance matrices in ERALIB1 and JECCOLIB2 should therefore be further investigated to determine their range of validity, and assess whether the 15-group structure is suitable for the analysis of gas-cooled reactors.

For the reactivity coefficients, delayed neutron fraction and total breeding gain the fact that no significant discrepancy was highlighted, is likely the result of compensating effects.

6. Conclusions and prospects

The first phase of a neutronic benchmark based on the 2400 MWth gas cooled fast reactor design has been described. Four institutions took part in the analysis, by using two code systems (deterministic ERANOS and stochastic OCTOPUS). The nuclear data was primarily based on the JEF-2.2 evaluated nuclear data file, adjustments being accounted for in the ERANOS library ERALIB1. A comparison has been carried out for the following parameters: reactivity, Doppler effect, core depressurization reactivity, delayed neutron fraction and total breeding gain, calculated for both BOL and EOL conditions.

Initially a large discrepancy was observed between the results for the reactivity of the different participants, but after appropriate corrections the results showed a good agreement, i.e. within 62 pcm at BOL and within 178 pcm at EOL. In fact, parametric calculations indicate that the computed reactivity is particularly sensitive to the fission product treatment,

the number of burnup zones used in the radial direction, and to the specific data library. The lumped fission products currently available in the ERANOS libraries have to be re-evaluated for GCFR applications.

The other parameters being studied, viz. delayed neutron fraction, Doppler and depressurisation effects, as well as breeding gain, are found in good agreement without any correction. These findings underline the usefulness of these kinds of studies, especially in the pre-conceptual design phase of a new reactor. In the next benchmark phases, the reactor model will be gradually refined (see Section 2).

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