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ALFRED Reactor: evaluation of multi temperature cross section sets by deterministic and stochastic methods

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ALFRED REACTOR: EVALUATION OF MULTI TEMPERATURE CROSS SECTION SETS BY DETERMINISTIC AND STOCHASTIC METHODS

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Il presente documento descrive le attività di ricerca svolte all'interno dell'Accordo di collaborazione "Sviluppo competenze scientifiche nel campo della sicurezza nucleare e collaborazione ai programmi internazionali per il nucleare di IV generazione"
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Sommario

Nel presente rapporto viene descritta la metodologia adottata per condensare sezioni d'urto, con riferimento al reattore ALFRED, per valutarne transitori operazionali e incidentali. Le temperature del combustibile (ossidi misti) e del refrigerante (piombo) sono utilizzate come parametri. La libreria usata è la JEFF 3.1; partendo dalla struttura a 1968 gruppi, si arriva ad una a 5 gruppi. È stato utilizzato il codice francese ERANOS (modulo ECCO). Sono riportati altresì alcuni calcoli di flusso, sul reattore, utilizzando il modulo VARIANT, per un test sulla coerenza dei dati ottenuti. La valutazione delle sezioni d'urto è stata inoltre svolta con un approccio statistico utilizzando il codice Monte Carlo SERPENT.

Note

Lavoro in collaborazione con Politecnico di Torino (POLITO) e Università di Roma (La Sapienza)

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1. Introduction

ALFRED program (Advanced Lead-cooled Fast Reactor European Demonstrator) [1] is in the framework of the LEADER project (EURATOM VII Framework Programme) [2]. The aim of ALFRED is to analyze the various aspects of the technology of the lead cooled fast reactors.
It thus can play a very important role as ETDR (European Technology Demonstrator Reactor) in the overall technology chain.
This document describes the methodologies used to evaluate the cross sections sets, from the Library JEFF3.1, and from many energy groups (1968), collapsed on five groups, on the structures (core, reflector, safety and control rods) of ALFRED reactor. Those sets have been evaluated on different fuel and coolant (lead) temperatures (from the library), by using the module ECCO of the ERANOS French code. The need to have many sets at different fuel and coolant temperatures comes from the need to analyze several operational and accidental transient situations.
Besides, some reactor calculations have been made, by using different sets of cross sections at different temperatures, to evaluate the consistency of data just got. We used a module of ERANOS, named VARIANT, a transport, 3D (here used in hexagonal-z), coarse mesh, code.

2. ALFRED System, a Short Description.

ALFRED (Advanced Lead-cooled Fast Reactor European Demonstrator) is a demonstrator of the lead fast reactor technology, with a foreseen thermal power of 300 MW. Some indicative parameters of the ALFRED reference geometry used in this work have been reported in Table **1**: the core has a hexagonal lattice composed by 171 fuel assemblies (FA), 12 control rods (CR), 4 safety rods (SR) and 108 dummy elements, as shown in Figure 1.

Table 1
Main Parameters of the Alfred Reactor.

Parameter	Unit	Values
Thermal power	MW	300
Active height	cm	60
Pellet hollow diameter	mm	2
Pellet radius	mm	4.5
Gap thickness	mm	0.15
Clad thickness	mm	0.6
Pin diameter	mm	10.5
Wrapper thickness	mm	4
Distance between 2 wrappers	mm	5
Coolant velocity	m s^{-1}	~1.4
Lattice pitch (hexagonal)	mm	13.86
Pins per FA	-	127
Inner vessel radius	cm	165

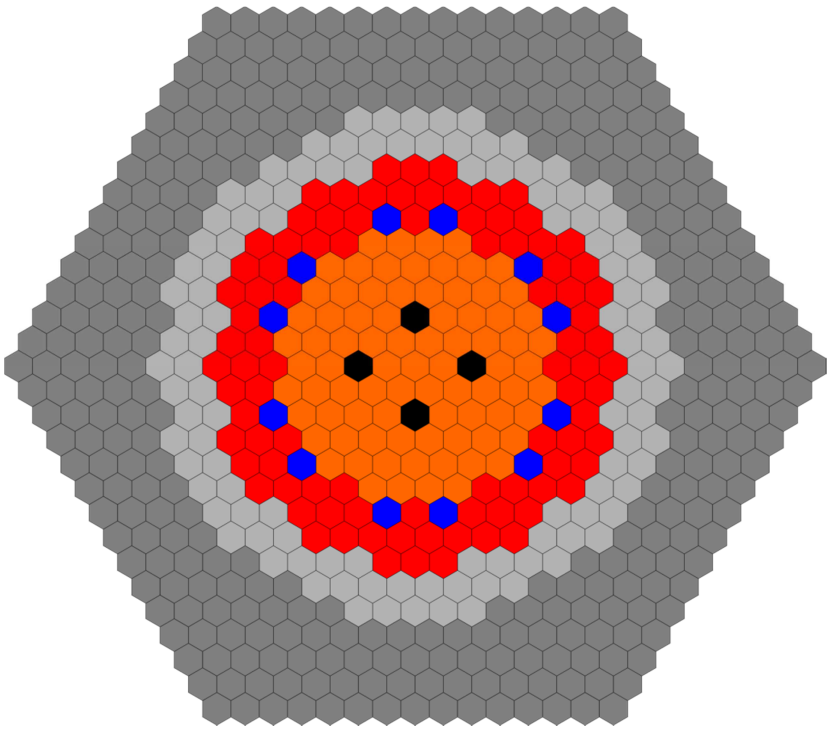


Figure 1
Scheme of the two enrichment zones of the core (orange and red positions), of control (blue) and safety (black) rods and the reflector elements (light gray).

The composition of U and Pu vectors is a typical MOX fuel but the enrichment is different for inner (orange FA) and outer (red FA) core zones; it is approximately 20-30% of Pu+Am/Pu+Am+U respectively for inner and outer fuel, as reported in [1].
The fuel assembly is composed of 127 fuel pins and a stainless steel hexagonal box; it is cooled by lead. An ERANOS scheme is shown in Figure 2.
For both control and safety rods the absorbing material is B_4C (with 90% at ^{10}B) with density 2.2 g/cm^3.
The safety rods are made of a cylindrical bundle of 12 absorbing pins and a stainless steel box, as shown in Figure 3. The rods are also cooled by primary lead, and are inserted from the top of the reactor and positioned in the core map shown in Figure 1 (black positions).
The control rods are similar to safety rods, they have only 19 bundled pins of absorbing material with a stainless steel casing and cooled by primary lead, and they are inserted from the core bottom part (Figure 4).

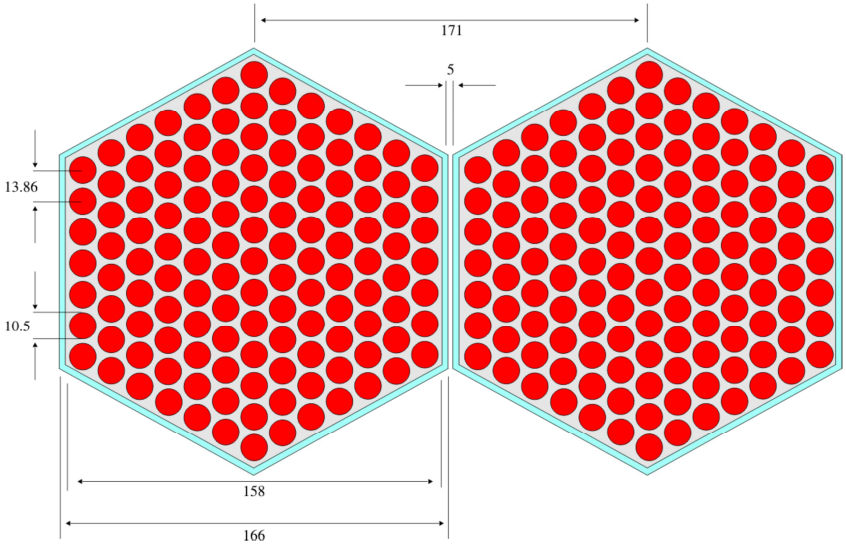


Figure 2
Fuel Assembly Scheme.

An axial overview of the system is shown in Figure 5, in which the main parts of the reactor considered for this analysis are presented.

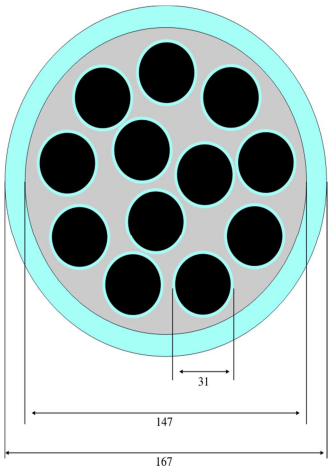


Figure 3
Safety rods scheme. To notice the 12 absorbing pins.

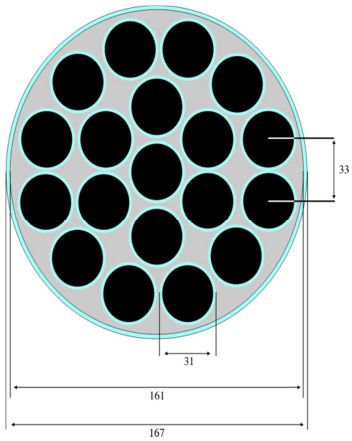
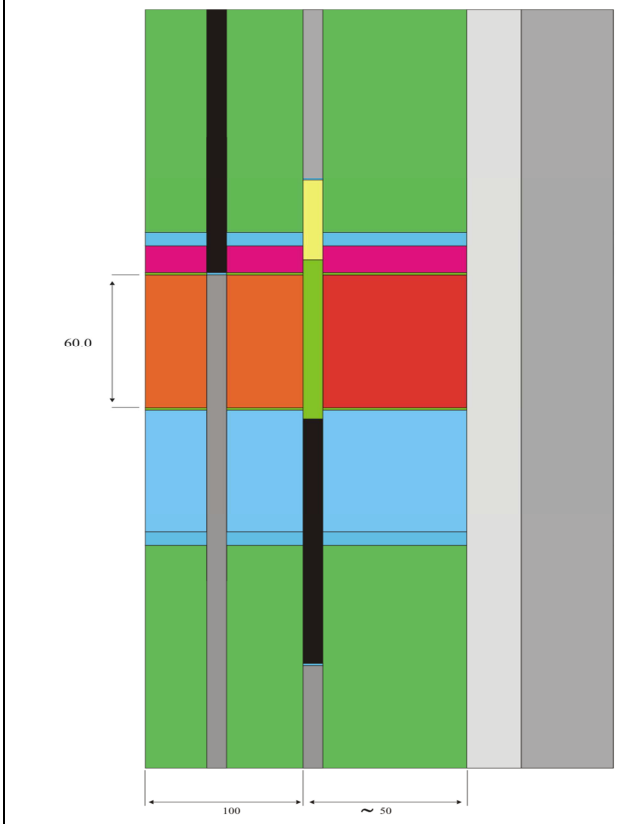


Figure 4
Control rods scheme (19 absorbing pins).

Figure 5
A simplified axial scheme of the Alfred reactor.



Starting from the top of the sketch, the upper reflector, modeled as made by lead only, is reported as a green zone, then the upper part of the different elements, are respectively in blue and pink. Then we have two different fuel zones (orange and red in figure) with 60 cm active length; 1 cm thermal insulator is set at the upper and the bottom of the core. In the bottom part, after the plenum zones, there are the same structures described at the top. At the end on the right of the scheme there are the dummies assemblies, in light gray, and the outer reflector, in dark gray; both are modeled as made by lead.

3. The ERANOS code.

The European Reactor Analysis Optimized calculation System, ERANOS, has been developed and validated with the aim of providing an appropriate basis for neutronic calculations of current fast (and thermal) reactor cores. It consists of data libraries, deterministic codes and calculation procedures developed within a European framework and it meets the needs expressed by the industrialists and the teams working on the design of fast reactors, present and future.
ERANOS is written using the ALOS software which requires only standard FORTRAN

compilers and include advanced programming features. It allows, with the use of LU user's language, to perform programs of R&D in reactor physics without needing specific development.

3.1 Architecture.

Fast reactor core, shielding and fuel cycle calculations can be performed with the ERANOS system. A modular structure was adopted for easier evolution and incorporation of new functionalities.
Blocks of data can be created (data SETs) or used by different modules or by the user with LU control language. Programming and dynamic memory allocation are performed with the use of the ESOPE language. It can be possible to make an external temporary storage or permanent storage with the GEMAT and ARCHIVE functions, respectively. ESOPE, LU, GEMAT, and ARCHIVE are all part of the ALOS software.
This type of structure, based on a modular system, allows to link together different modules in procedures corresponding to recommended calculation routes ranging from fast-running and moderately-accurate 'routine' procedures to slow-running but highly-accurate 'reference' procedure.
The main contents of ERANOS-2.1/2.2 package are:

- nuclear data libraries, multigroup cross sections from ERALIB1, ENDF-/B-VI.8, JEFF-2.2, JEFF-3.1 evaluated nuclear data files, and other specific data;
- a cell and lattice code, ECCO;
- reactor flux solvers (diffusion, S_n transport, nodal variational transport);
- a burn-up module;
- different processing modules (material and neutron balance, breeding gains,…);
- perturbation theory and sensitivity analysis modules;
- core follow-up modules;
- a fine burn-up analysis subset named MECCYCO (mass balances, activities, decay heat, dose rate).

Each nuclear data package contains four neutron cross section libraries obtained by processing the corresponding nuclear data files by the NJOY and CALENDF codes and they are:

- a 1968 energy group library containing 41 main nuclides;
- a 33 energy group library containing 246 nuclides, including pseudo fission products;
- a 175 energy group library used for shielding calculation only;
- a 172 energy group library used mainly for thermal spectrum calculations.

3.2 Cell Calculations

The ERANOS code has been developed within the European Collaboration on Fast Reactors over the past 30 years or so. It consists of data libraries, deterministic codes and calculation procedures.
ERANOS is a deterministic code system, by which neutron physics calculations are performed at the cell/lattice level and at the core level. The development of the ECCO Code was decided in 1985 by several R&D teams working within the framework of the European Fast Reactor Collaboration [3].
ECCO [4], European Cell COde, is the cell code allowing to calculate the cross sections matrices to be used in spatial core calculations performed by different ERANOS modules.
First of all, it is necessary to provide to ECCO media composition (homogeneous mixtures), expansion coefficients and geometric description of the cell. Then the cross sections are calculated by using the defined media and the associated nuclear data libraries by means of the collision probability method. The nuclear data libraries are available at different temperature (293.6, 573.6, 973.6, 1473.6, and 2973.6 K) to take into account the Doppler Effect for the main nuclides.
An ECCO calculation corresponds to a succession of STEPs, and for each STEP one can select energy structure, cell geometry (heterogeneous or homogeneous), flux calculation type, and so on.
Many type of geometry are available within the ECCO code:

- 1D, plane or cylindrical calculated by exact collision probabilities method;
- 2D, rectangular lattice made of cylindrical and/or square pins within a square tube, hexagonal lattice made of cylindrical pins within a hexagonal sheet calculated by approximate collision probability method (Roth and double step methods);
- 3D, XYZ and HEX-Z calculated by approximate collision probability method.

The user has the possibility to chain several calculation steps so as to produce design or reference calculations, or even to use specific capabilities, according to the need of the study.
The module ECCO has some procedures to carry out the calculations; those have been named “route”. The first route is the “reference” one: it does not care about the calculation time and treats the heterogeneous cell at fine energy group level (1968 groups). The second route is the “project” or “design” one in which some simplifying hypotheses are assumed, the elastic slowing down is treated in a homogeneous geometry but at fine group level, the self-shielding is treated in a heterogeneous geometry at broad group level (33 groups).

3.3 Static Calculations.

ERANOS allows several types of flux calculations: diffusion and transport calculations with different methods; in each case can be addressed external source, up-scattering and adjoint calculations. For all geometries, 1D plane, cylindrical and spherical, 2D RZ, R-theta, rectangular lattice XY, hexagonal lattice, and 3D rectangular lattice XYZ, hexagonal-Z, can

be used finite difference diffusion solvers. In 1D and in some 2D geometries, like RZ and XY, finite difference S_n transport calculations can be performed by means of the BISTRO [5] code. The physics of thermal and fast reactors require the capability to solve the transport equation in accurate manner for different 2D and 3D geometries; variational nodal methods are well adapted for these topics because of the reduced numbers of unknowns used and the good accuracy in the solution by using high order approximation for spatial and angular expansions of flux and current in the node.
Both 2D (XY and hexagonal) and 3D (XYZ and hexagonal-Z) geometries are available within the TGV/VARIANT [6] variational nodal module. The module performs direct flux calculations, with and without an external source, and adjoint calculations, and it is possible to set up several parameters for different types of analyses. The computing time, in comparison with other methods devoted to the transport equation solution (like S_n), is very competitive.

4. Calculation Methods: Energy Structure, and Selected Temperatures.

This work is focused on the analysis of the multi-temperature cross sections for the ALFRED reactor. The basic library for the nuclear data utilized for these calculations is JEFF-3.1.
An energy structure composed by 5 energy groups has been chosen to carry out the cell calculations to obtain the cross sections; the upper energy limits are presented in Table 2. This energy structure has been chosen taking into account the principal neutronic aspects of the main components of the system (MOX and lead) and has been derived from the standard energy structure at 1968 groups, after some preliminary studies that will not be mentioned in this work.

Group	Upper Energy (eV)
1	1.9640E+07
2	1.3534E+06
3	1.8316E+05
4	6.7379E+04
5	9.1188E+03

Table 2
Energy Structure.

ECCO cell calculations, with different temperature conditions, have been carried out in different way for each component; the influence of the Doppler effect has been taken into account for all the structures of the system while the dilatation coefficients have been considered only for the coolant.
The temperatures chosen are different for the core analysis and for other components:

1- the core analysis, both for fuel and lead, was carried out at different temperatures, the same temperatures available in the nuclear data of the basic library JEFF-3.1, as reported in the previous chapter (293.6, 573.6, 973.6, 1473.6, 2973.6 K);
2- the other components: control rods, safety rods, reflector, upper and bottom part of the system have been evaluated at 673.6 K, the coolant inlet temperature;
3- the dummy elements have been evaluated at 713.6 K, the coolant core average temperature.

5. Reactivity Test Analysis.

Some TGV-VARIANT flux calculations have been done, with cross sections evaluated at different temperatures, to check how consistent the multi-temperature cross sections are.
The results of k_{eff} are presented in Table 2; the temperatures of fuel and lead for each calculation, in Kelvin, and the reactivity in pcm are provided. The first set of results has been obtained increasing the fuel temperature and maintaining steady the coolant temperature, in the second part of the table the fuel temperature is steady and the lead temperature increases.

Fuel T(K)	**Lead T(K)**	**k_{eff}**	**ρ (pcm)**
293	293	1.09337	8540
973	293	1.08650	7961
1973	293	1.08287	7653
2973	293	1.08093	7487
2973	973	1.08080	7476
2973	1473	1.08102	7495
2973	1973	1.08132	7520
2973	2973	1.08202	7580

Table 3
K_{eff} and Reactivities Values Depending on Fuel and Lead Temperatures.

It can be noticed that, when the fuel temperature increases and the temperature of the coolant remains constant, the reactivity of the system decreases because of the Doppler effect.
In the second part of the Table 3, when the fuel temperature is constant and the lead temperature is increasing, there is an opposite behavior of the k_{eff} value compared to the previous case: both reactivity and lead temperature increase.
In this situation we should have two effects: a lower density of the lead causes a decrease of the neutron population because of leakage; on the other hand a decrease of the moderating effect with the consequent lower slowing down, implies an increase of the fast neutrons. Following the k_{eff} results, the last effect seems to be more important. Other specific

calculations should be needed, as perturbative ones, to analyze more deeply those effects and their combination.

6. ERANOS cross section results.

The results are the multi-temperature macroscopic cross sections for the ALFRED structures. First of all the analysis for the core lattice has been carried out considering the fuel temperature from 293.6 K to 2973.6 K, as said before. In special way we considered only the cases in which the lead temperature is less or equal and never greater than that of the fuel. All other assembly structures have the same fuel temperature.
Upper and bottom lead reflectors have been analyzed for the same temperatures used for the previous core analysis (293.6, 573.6, 973.6, 1473.6, 2973.6 K), to get a better evaluation of the neutronic lead behavior.
Then the temperatures considered for the dummy elements and the other components are those explained in chapter 4.
The macroscopic cross sections for the main nuclear reactions are:

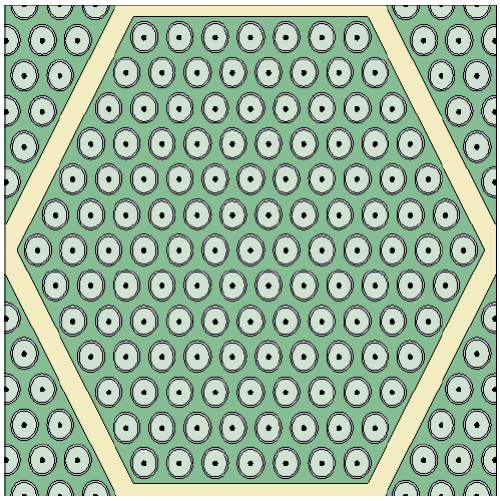
1. Capture,
2. Fission,
3. NU*Fission;
4. Disappearance (sum of: capture, fission, N-XN, inelastic, elastic cross sections; minus: inelastic cross section in the same group);
5. Elastic;
6. Inelastic;
7. N, XN;
8. Matrix Scattering.

7. Cross section evaluation by the Monte Carlo SERPENT code

At Politecnico di Torino, the generation of the energy spectrum used for collapsing the nuclear parameters into a few groups set has been performed by the Monte Carlo SERPENT code [7-8]. The spectrum is generated over a single fuel element in the real geometrical detail and the averaging procedure leads to homogenized parameters for a defined energy group structure.
To this work the student Carles Garcia Domínguez has significantly collaborated in the frame of the preparation of his Master's thesis, during an ERASMUS exchange period spent at Dipartimento Energia of Politecnico di Torino [9].

The configuration is assumed consistent with the actual design of the ALFRED core as proposed within the European Project LEADER. The fuel element is designed in hexagonal shape and it is schematically represented in Fig. 2. For the SERPENT spectrum calculations, the geometrical configuration adopted is reported in Fig. 6. Reflective boundary conditions are assumed on the external boundary and thus an infinite lattice assumption is made.

Figure 6
SERPENT geometrical configuration.

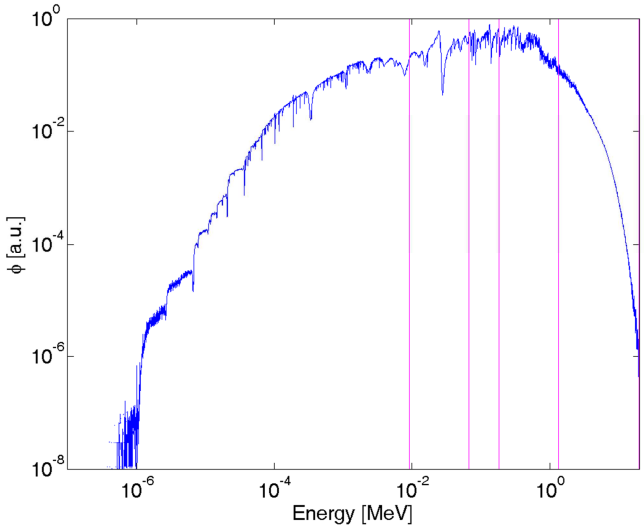


SERPENT is a Monte Carlo code specifically developed in the past 6 years for reactor physics-related applications. In particular, the code is well suited to perform cell calculations to the aim of producing homogenized, few-group cross sections to be used in full-core simulation. Therefore, the cross sections generated within this project can be profitably used to perform coupled neutronic and thermal-hydraulic calculations with the code FRENETIC, currently being developed at Politecnico di Torino [10].
The calculation of the 5-group cross sections has been performed adopting the same energy discretization as presented in Table 2. The fuel and coolant temperatures have been parameterized according to the values available in the SERPENT library (600 K, 900 K and 1200 K), in order to obtain a cross section database with a similar structure to the one evaluated with ERANOS. Obviously the fuel temperature has always been considered larger, or equal, to the coolant temperature.
The energy spectrum in the fuel assembly as obtained with the SERPENT code is reported in Fig. 7, where the energy cutoff adopted for the generation of multigroup parameters are also highlighted. The cross sections evaluated with SERPENT are summarized in Table 4.

Symbol	Definition	Units
Σ_t	Total cross section	[cm^{-1}]
Σ_a	Absorption cross section	[cm^{-1}]
Σ_f	Fission cross section	[cm^{-1}]
$\nu\Sigma_f$	Fission cross section × mean number of fission neutrons	[cm^{-1}]
Σ_c	Capture cross section	[cm^{-1}]
Σ_s	Total scattering cross section	[cm^{-1}]
D	Diffusion coefficient	[cm]
1/v	Inverse of neutron velocity	[s/cm]
Σ_r	Removal cross section	[cm^{-1}]
$\Sigma_{g' \to g}$	Scattering cross section from group g' to group g	[cm^{-1}]

Table 4. Cross sections evaluated by SERPENT code.

Figure 7
Energy spectrum in the LFR fuel assembly evaluated by SERPENT code.



8. Conclusions.

In the frame of the ALFRED project, the aim of the activity illustrated in this report was to prepare a given number of cross sections sets from the library at 1968 groups library JEFF 3.1. All the sets are evaluated at different fuel and coolant temperatures, to cover every situation the system can reach during operation and accidental transients. The chosen energy structure, after some tests not reported here, was at five groups. The calculations were made by the cell code ECCO, a module of the code ERANOS, and the Monte Carlo code SERPENT. At last a series of reactor (flux) calculations were made, by using another ERANOS module (transport, hexagonal-z, broad meshes) named Variant. An inter comparison among the resulting reactivity values, shows some effects not completely

explained in the present work. Additional analysis (for example perturbative calculations) could be desirable.

9. References.

1) G. Grasso et al. Demonstrating the effectiveness of the European LFR concept: the ALFRED core design. In Proceedings of *Fast Reactors and Related Fuel Cycles: Safe Technologies and Sustainable Scenarios (FR13)*, Paris, March 4-7 2013, IAEA, Vienna.

2) Lead-cooled European Advanced DEmonstration Reactor (LEADER) – Annex I "Description of Work", Grant agreement no. FP7-249668 (3 May 2010), Rev. 0.

3) "Methods for Reactor Physics Calculations for Control Rods in Fast Reactors", IAEA, Winfrith, UK, 6-8 December 1988 - IWGFR/69, IAEA, Vienna, 1990.

4) G. Rimpault, "Physics documentation of the ERANOS. The ECCO cell code", CEA Technical Note RT-SPRC-LEPh-97-001, 1997.

5) C.J. Gho, G. Palmiotti, "BISTRO: Bidimensional S_n TRansport Optimise. Un programme bidimensionnel de transport S_n aux differences finies. Note n°1. Definition des algorithms pour la geometrie X-Y", CEA Technical Note NT-SPRC-LEPh-84-270, 1984.

6) G. Palmiotti et al., "Variational Nodal Method for the Solution of the Diffusion and Transport equation in two and three dimensional geometries", CEA Technical Note NT-SPRC-LEPh-91-208, 1991.

7) J. Leppänen, *Development of a new Monte Carlo reactor physics code*, PhD Thesis, VTT Technical Research Center of Finland, Helsinki, 2007.

8) E. Fridman, J. Leppänen, On the use of the Serpent Monte Carlo code for few-group cross section generation, *Annals of Nuclear Energy*, **38**, 1399-1405, 2011.

9) C. Garcia Domínguez, *Generation of nuclear data for Lead-cooled Fast Reactor using the Monte Carlo method*, Master's thesis, Politecnico di Torino, Torino,. 2013.

10) R. Bonifetto, S. Dulla, P. Ravetto, L. Savoldi, R. Zanino, A full-core coupled neutronic/thermal-hydraulic code for the modeling of lead-cooled nuclear fast reactors, *Nuclear Engineering and Design*, **261**, 85-94, 2013.