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MACROSCOPIC MULTIGROUP CONSTANTS FOR ACCELERATOR DRIVEN SYSTEM CORE CALCULATIONS

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ABSTRACT

The high-level wastes stored in facilities above ground or shallow repositories, in close connection with its nuclear power plant, can take almost 10^6 years before the radiotoxity became of the order of the background. While the disposal issue is not urgent from a technical viewpoint, it is recognized that extended storage in the facilities is not acceptable since these ones cannot provide sufficient isolation in the long term and neither is it ethical to leave the waste problem to future generations. A technique to diminish this time is to transmute these long-lived elements into short-lived elements. The approach is to use an Accelerator Driven System (ADS), a sub-critical arrangement which uses a Spallation Neutron Source (SNS), after separation the minor actinides and the long-lived fission products (LLFP), to convert them to short-lived isotopes. As an advanced reactor fuel, still today, there is a few data around these type of core systems. In this paper we generate macroscopic multigroup constants for use in calculations of a typical ADS fuel, take into consideration, the ENDF/B-VI data file. Four energy groups are chosen to collapse the data from ENDF/B-VI data file by PREPRO code. A typical MOX fuel cell is used to validate the methodology. The results are used to calculate one typical subcritical ADS core.

KEYWORDS: ADS, Transmutation, Fertile-Free Fuel, Data File, Cell Calculations.

1. INTRODUCTION

A technique to diminish this time is to transmute these long-lived elements into short-lived elements [1]. The approach is to use an Accelerator Driven System (ADS), a sub-critical arrangement which uses a Spallation Neutron Source (SNS) [2,3], after separation the minor actinides and the long-lived fission products (LLFP), to convert them to short-lived isotopes.

The facilities for transmutation are envisaging to use some Minor Actinides (MAs) as fertile-free fuel, like $(Pu_{0.4}, Am_{0.5}, Cm_{0.1})O_{2-X} - Mo$ [4], because of their neutronic qualities. However, macroscopic cross section of this fuel material still presents some challenge because they belong to an new concept on reactor cores.

The generation of macroscopic constants for calculations of reactor cores has a significant impact in defining the core and shielding calculations. The SCALE code [1,5] represents the

state of the art regarding the latest platforms reactor core calculations, since the generation of cross sections of neutrons and their spectra, through the cell calculations and criticality. SCALE, besides dealing with classic materials of various concepts of existing reactors, also includes materials that are being seen as candidates for the concepts of the next generation of reactors. Due to its modularity, code has a broad range of applications, and only one, its use is subject to license, usually tied to a single computer. This affects the researcher to be associated with large groups or research centers, to benefit from such tools. HAMMER code [2,6] and their versions for many years, represented an alternative to the majority of the community who deal with data and nuclear cross sections. HAMMER code does not cover a wide range of materials that had gained importance in recent years, as the Minor Actinides (MAs), transmutation reactor studies. Therefore, for any conceptual calculation of nuclear reactor analysis, be it a current or innovative one, the starting point to obtain preliminary results,, we need, first of all, an updated library of nuclear data.

This paper presents a methodology to generate macroscopic multigroup constants for use in calculations of a typical ADS fuel, take into consideration the ENDF/B-VI data file [7]. The application uses four energy groups of data collapsed from ENDF/B-VI file, a part from PREPRO code [8]. A typical MOX fuel cell is used to validate the methodology [9]. The results are used to calculate one typical subcritical ADS core, based on CINESP codes [10,11]. The codes are used to calculate, first, a subcritical configuration (CINESP). Then, CNESP-ADS is used to calculate the flux distribution [12]. In both we have used the group constants modeled in this paper.

2. METHODOLOGY

2.1. Few Groups Generation from ENDF/B

From ENDF/B-VII files, we use the following algorithm to obtain the neutron cross sections : for each isotope in list1, we do for each temperature in list2 and then, we execute the LINEAR program, converting evaluated cross sections in the ENDF/B format into a tabular form. That is subject to linear-linear interpolation in energy and cross section, and out putting the result in the ENDF/B format. Then, we execute RECENT. This program is designed to reconstruct the resonance contribution to the cross section in a linearly interpolable form, add it up any linearly interpolable background cross section, out putting the result in the ENDF/B format. The cross sections output by this program are linearly interpolable over the entire energy range. After that, we execute SIGMA1. This program is designed for broadening the Doppler resonance cross sections induced by neutron. It also out puts the result in the ENDF/B format. The ACTIVATE program is run to create file 10 activation cross sections by combining file 3 cross sections and file 9 multipliers, and out puts the result in the ENDF/B format, too. Following, LEGEND program is run to calculate linearly interpolable, tabulated angular distributions, starting from data in the ENDF/B format. In the sequence, FIXUP is executed. This program is designed to read evaluated data in the ENDF/B format, to perform corrections, and to out put the result in the ENDF/B format. Now, GROUPIE is executed. This program is designed to calculate any combination of unshielded group averaged cross sections; Bondarenko self-shielded group averaged cross sections and or multi-band

parameters from linearly interpolable tabulated cross sections in the ENDF/B format [13]. Finally, a tabulated cross section data is read by a properly program, nominated freely.

2.2. Cell Calculations

For a cell composed by fuel region (F), cladding (C) and the coolant (M) [14],

$$\Sigma_{xg}^{cell} = \frac{\Sigma_{xFg} + \zeta_{Cg}\frac{V_M}{V_F}\Sigma_{xCg} + \zeta_{Mg}\frac{V_M}{V_F}\Sigma_{xMg}}{1+\zeta_{Cg}\frac{V_C}{V_F}+\zeta_{Mg}\frac{V_M}{V_F}}, \tag{1}$$

where,

$$\zeta_{Mg} = \frac{\overline{\varphi}_{Mg}}{\overline{\varphi}_{Fg}}, \tag{2}$$

$$\zeta_{Cg} = \frac{\overline{\varphi}_{Cg}}{\overline{\varphi}_{Fg}}, \tag{3}$$

$x = capture, scattering, fission, etc.$
Since,

$$\Sigma_{xyg}^{i} = \rho_y \frac{N_0}{A_y^i}\sigma_{xyg}^{i}, \tag{4}$$

$\rho_y =$ material density at region y weight percent in the mixture of isotopes,

$N_0 = 6.022x10^{23} =$ Avogadro's number,
$\sigma_{xyg}^{i} =$ group cross section for reaction x of the nuclide i in region y,

$A_y^i =$ Atomic or molecular number associated with i, at region y.

With that we have:

$$\Sigma_{xyg} = \sum_{i=1}^{m}\left(\omega_{yi}\Sigma_{xyg}^{i}\right), \tag{5}$$

where,

$\omega_{yi} =$ fraction of the isotope i in the mixture, in region y.

The coupled down scattering cross sections are given by [14]:

$$\Sigma^{i}_{syg\to g+1} = \frac{\overline{\xi}^{i}_{yg}\Sigma^{i}_{syg}}{\Delta u_g}, \tag{6}$$

where,

$$u_g = \ln\frac{E_0}{E_g}, \tag{7}$$

is the lethargy, and

$$\Delta u_g = u_{g-1} - u_g \quad g = 1,2,3,...,G. \tag{8}$$

$$\xi^{i}_{y} = \frac{2}{A^{i}_{y} + \frac{2}{3}}, \quad A^{i}_{y} >> 1, \tag{9}$$

$$\overline{\xi}^{i}_{yg} = \frac{\sum_{i}\Sigma^{i}_{syg}\xi^{i}_{y}}{\sum_{i}\Sigma^{i}_{syg}}, \tag{10}$$

The diffusion coefficients are calculated apart from:

$$\Sigma_{tg} = \sum_{x}\Sigma_{xg}, \tag{11}$$

$$\Sigma_{tryg} = \Sigma_{tyg} - \overline{\mu}_{y}\Sigma_{syg}, \tag{12}$$

$$\overline{\mu}_{y} = \frac{2}{3A_{y}}. \tag{13}$$

Finally,

$$D_g = \frac{1}{3\Sigma_{trg}}. \tag{14}$$

2.3. Subcritical Configuration

The methodology to be used in this analysis consists in, given the energy groups and multigroup constants, determining the ADS dimension, whose effective multiplication factor $\kappa_{eff} < 1$, i.e., an arrangement between composition and geometry that holds the core sub-critical. In this way, we use the criticality equation for a critical system given by [15]:

$$-\nabla \cdot D_g \nabla \varphi_{kg} + \Sigma_{Rg}\, \varphi_{kg} = \sum_{g' \neq g}^{G} \Sigma_{sg'g}\, \varphi_{kg'} + \frac{\chi_g}{\kappa_{eff}} \sum_{g'=1}^{G} \nu_{g'}\, \Sigma_{fg'}\, \varphi_{sg'}\,, \quad g = 1,2,...,G\,, \tag{15}$$

where, φ_{kg} is the sub-critical neutron flux of energy group g. Since k_{eff} is set, the reactor dimensions are adjusted, solving Eq. (15), until that one matches with k_{eff}.

2.4. Flux Distribution for an External Neutron Source

From core dimension setting, we solve the Eq. (15), now using the external neutron source S intensity to sustain the neutronic balance. With that, we have [15]:

$$-\nabla \cdot D_g \nabla \varphi_{Ng} + \Sigma_{Rg}\, \varphi_{Ng} = \sum_{g' \neq g}^{G} \Sigma_{sg'g}\, \varphi_{Nkg'} + \chi_g \sum_{g'=1}^{G} \nu_{g'}\, \Sigma_{fg'}\, \varphi_{Ng'} + \chi_{sg} S\,,\ g = 1,2,...,G\,, \tag{16}$$

where, φ_{Ng} now is the nominal neutron flux of energy group g, associated with the external neutron source S. The spallation neutron spectrum is such that:

$$\sum_{g=1}^{G} \chi_{sg} = 1. \tag{17}$$

3. NUMERICAL DISCRETIZATIONS

Equations (15) and (16) are discretized in space using the box integration scheme, with mesh centered in the interface and having in mind a 2D grid in a spatial variables x and y. A parameter α is introduced to represent the diffusion operator in Cartesian ($\alpha = 0$) and Cylindrical ($\alpha = 1$) geometries. The symbolic integrations are given by:

$$T_{gij} = \int_{y_j - \frac{\Delta y}{2}}^{y_j + \frac{\Delta y}{2}} dy \int_{x_i - \frac{\Delta x}{2}}^{x_i + \frac{\Delta x}{2}} x^{\alpha} dx R_g(x,y) H_g(x,y)\,, \tag{18}$$

Where T_{gij} are generic terms associated with the variables $H_g(x,y)$ representing the fluxes given in Eq. (15) and Eq. (16). When it is the case, parameters $R_g = R_g(x,y)$ can represent properties like Σ_{xg}, S_g, etc., where x means reaction types.

The above integration leads to following matricidal equation:

$$\underline{\underline{M}}\,\underline{\psi} = \underline{S}\,, \tag{19}$$

where $\underline{\psi}$ and $\underline{S}$ are vectors given by:

$$\underline{\psi} = col\left\{\varphi_{111}, \varphi_{121}, ...\varphi_{112}, \varphi_{122}, ...\varphi_{gij}, ..., \varphi_{GLN}\right\}, \tag{20}$$

$$\underline{S} = col\left\{\chi_{s1}S_{11}, \chi_{s1}S_{21}, ...\chi_{s1}S_{12}, \chi_{s1}S_{22}, ...\chi_{sg}S_{ij}, ..., \chi_{sG}S_{LN}\right\}, \tag{21}$$

and $\underline{\underline{M}}$ is a matrix associated with the spatial discretization of Eq. (15) or Eq. (16).

The solution of Eq. (19) is given by:

$$\underline{\psi} = \underline{\underline{M}}^{-1}\underline{S}, \tag{22}$$

As $\underline{\underline{M}}$ is a sparse matrix, the classic iterative method Successive Over-Relaxation (SOR) is used to obtain $\underline{\psi}$.

4. RESULTS

4.1. Methodology Validation

The PREPRO Code, which generates the few group constants, was validated for some nuclides found in the literature [16], taking $G = 4$, for comparison. To achieve four group neutron microscopic cross sections, we adopted the region threshold in 0.2 eV, 15KeV, 100KeV, 820KeV and limit energy of 20MeV. We generate the natural concentration of all isotopes in this work and as well as the macroscopic cross section used in cell calculation. Tables II, III and IV show the transport, fission and capture microscopic cross sections from literature, first column (in blue), and PREPRO methodology, second one (in black). Most of the data shows good agreement, especially regarding the magnitude of values. We must emphasize that the cutoff energies adopted in PREPRO are different in the ends, what could influence in some values.

Table II. Microscopic group $\sigma_{trg}(b)$

g	1		2		3		4	
Pu239	**4.9**	6.47	**7.5**	9.06	**12.0**	13.04	**17.4**	18.73
Pu240	**4.8**	6.46	**7.4**	9.09	**12.0**	12.63	**17.2**	17.96
Pu242	**4.5**	6.61	**7.1**	9.58	**12.6**	13.27	**22.0**	17.03
U235	**4.6**	6.41	**7.4**	8.73	**12.5**	12.94	**18.7**	18.18
U238	**4.6**	6.47	**7.8**	8.94	**18.7**	12.89	**12.9**	18.37
Cr	**2.4**	2.87	**3.6**	3.64	**4.5**	5.86	**11.1**	14.00
Fe	**2.2**	2.26	**2.8**	2.77	**5.1**	5.86	**7.2**	7.89
Bi	**-**	5.90	**-**	6.75	**-**	10.94	**-**	14.14
Ni	**2.3**	4.19	**4.4**	6.52	**12.7**	12.55	**21.1**	16.91
O	**2.2**	1.56	**3.8**	4.12	**3.6**	3.59	**3.6**	3.70
Pb	**-**	5.85	**-**	6.46	**-**	10.89	**-**	10.77

Table III. Microscopic group $\sigma_{fg}(b)$

g	1		2		3		4	
Pu239	**1.83**	2.160	**1.55**	1.572	**1.63**	1.564	**3.25**	3.188
Pu240	**1.59**	2.013	**.27**	0.476	**.07**	0.088	**.13**	0.108
Pu242	**1.46**	1.769	**.17**	0.301	**.04**	0.013	**.02**	0.017
U235	**1.2**	1.689	**1.3**	1.203	**1.9**	1.810	**5.0**	4.482
U238	**.32**	0.945	**0**	0.001	**0**	0.000	**0**	0.000

Table IV. Microscopic group $\sigma_{cg}(b)$

g	1		2		3		4	
Pu239	**.02**	0.0029	**.16**	0.1233	**.45**	0.3633	**2.4**	2.3056
Pu240	**.07**	0.0098	**.18**	0.1551	**.5**	0.5295	**2.1**	2.6523
Pu242	**.04**	0.0079	**.12**	0.1410	**.33**	0.4379	**1.54**	1.7970
U235	**.06**	0.0102	**.3**	0.1959	**.6**	0.5517	**2.0**	1.8406
U238	**.06**	0.0082	**.13**	0.1188	**.35**	0.3019	**.9**	1.4446
Cr	**.006**	0.0007	**.005**	0.0037	**.002**	0.0096	**.07**	0.0347
Fe	**.007**	0.0007	**.005**	0.0045	**.01**	0.0166	**.03**	0.0302
Bi	**-**	0.0008	**-**	0.0032	**-**	0.0020	**-**	0.0176
Ni	**.073**	0.0010	**.01**	0.0118	**.03**	0.0353	**.05**	0.4097
O	**.007**	0.0000	**0**	0.0000	**0**	0.0000	**0**	0.0000
Pb	**-**	0.0011	**-**	0.0042	**-**	0.0048	**-**	0.0115

4.2. The steady state flux distribution in an 1D ADS core

In Fig. 1 is sketched an ADS core, in 1D dimensional geometry, showing the fuel region and target one. Table VI and VII show the group constants, at fuel and target regions, considering 4 energy groups. With that, a search of sub-criticality was made, using CINESP Code in order to find a state where $K_{eff} = 0.9486428$, which implied a slab of 63.487cm, after 39 iterations and an accuracy of 10^{-6} for inner and outer iterations. In each fuel region and in the target one were used 35 and 10 meshes, respectively.

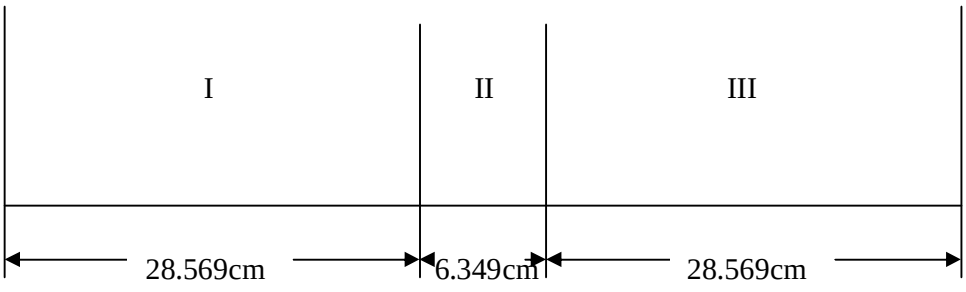

Figure 1. Slab dimension and source location.

4.3. Cell Composition

The cell composition contains the natural element composition: Uranium, Plutonium, Americium, Oxygen, Lead, Bismuth, at the following percent: 52.98/26.73/9.01/11.27/55.0/45.0.

The isotopic fuel composition is given in table V.

Table V. Fuel Composition.

U		Pu		Am	
Isotope	%	Isotope	%	Isotope	%
235	3.8	238	4.4	241	50.0
238	96.2	239	36.8	243	50.0
		240	15.7		
		241	11.0		
		242	21.2		

Table VI. Macroscopic group constants at cell region.

g	**1**	**2**	**3**	**4**
χ_g	**0.76**	**0.22**	**0.02**	**0.0**
χ_{sg}	**1.0**	**0.00**	**0.00**	**0.0**
ν_g	**4.4638**	**2.9044**	**2.8389**	**2.8327**
$\Sigma_{cg}(cm^{-1})$	$\mathbf{9.57x10^{-4}}$	$\mathbf{3.75x10^{-3}}$	$\mathbf{3.51x10^{-3}}$	$\mathbf{1.42x10^{-2}}$
$\Sigma_{fg}(cm^{-1})$	$\mathbf{2.98x10^{-3}}$	$\mathbf{8.06x10^{-3}}$	$\mathbf{7.1x10^{-3}}$	$\mathbf{1.731x10^{-2}}$
$\Sigma_{sg\to g+1}(cm^{-1})$	$\mathbf{1.21x10^{-5}}$	$\mathbf{5.71x10^{-5}}$	$\mathbf{1.05x10^{-4}}$	**-**
$D_g(cm)$	**1.84**	**1.64**	**0.989**	**0.878**

Table VII. Macroscopic group constants at target region.

g	**1**	**2**	**3**	**4**
$\Sigma_{cg}(cm^{-1})$	$\mathbf{1.79x10^{-2}}$	$\mathbf{1.11x10^{-2}}$	$\mathbf{1.36x10^{-2}}$	$\mathbf{3.51x10^{-2}}$
$\Sigma_{sg\to g+1}(cm^{-1})$	$\mathbf{2.38x10^{-4}}$	$\mathbf{1.37x10^{-3}}$	$\mathbf{2.20x10^{-3}}$	**-**
$D_g(cm)$	**2.09**	**1.66**	**1.08**	**0.640**

Following, CINESP-ADS was used to calculate the flux distributions, considering the external neutron source. Fig. 2 shows the normalized group fluxes. From figure we can see that the macroscopic multigroup cross section from our approach was adequate for use in an ADS core calculation.

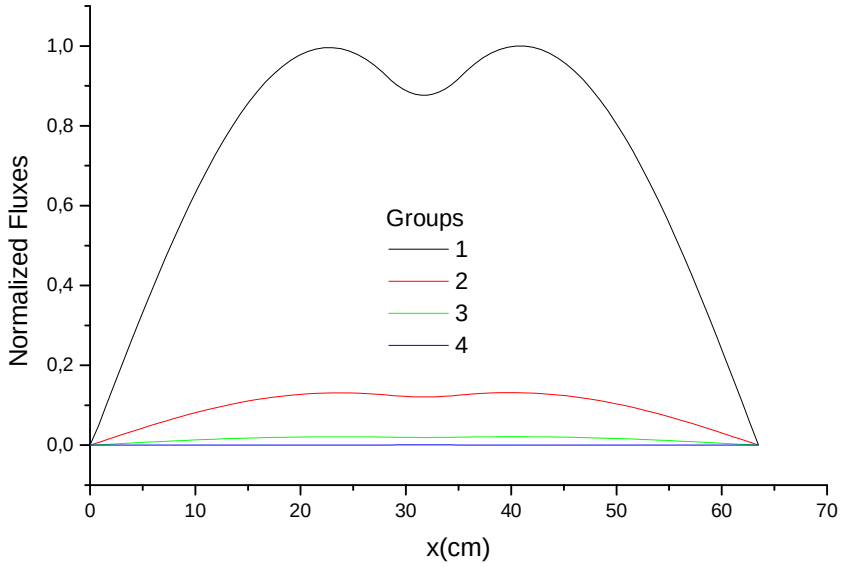

Figure 2. Neutron flux group distributions in 1D with the external source.

5. CONCLUSIONS

In this paper we have generated few group constants using code PREPRO by LLNL. This code have some limits, per example no produce the scattering matrices, however fit like a glove for this work. We use largely heavy metals with low inelastic scattering and suppose only one step scattering between energy groups.

This approach shown itself adequate for using in fast reactors, as the ADS, because its spatial and neutronic decoupling. Nowadays, most of evaluated nuclear data file are not update to deal with some nuclides envisaged to be used in an innovative systems. Results were compared with from carried like ADS. In our work we have applied our methodology for generic 1D ADS core calculations. The results showed adequate concordance with the physical behavior, as in the effective subcritical multiplication factor as in the neutron fluxes when driven by an external neutron source.

Resumming, we accomplished difficult and laborious isotopes like Cm, Am, Bi with poor descriptions in literature and all others like Fe, Mn, Mo , etc. From this blend, that comprises the problem kernel, has calculated a functional cell ADS reactor. In future we improve this methodology to attack complex cells with other toxic and long half-live materials .

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