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32.23 **STUDIEN ZUR AKTINIDENUMWANDLUNG**

32.23.05 **Untersuchungen zu beschleunigergetriebenen Systemen**

Generation of a Group Constant Library for Neutron Energy until 50 MeV. Tests and Applications

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Introduction:

Evaluated nuclear data libraries that are in use for the analysis of fission- and fusion- reactors (e.g. ENDF/B-VI, JEF2.2, JENDL3.2) cover the energy range from $1 \cdot 10^{-5}$ eV to 20 MeV. In accelerator driven systems the energies of the neutrons may reach several hundreds of MeV and even more than 1 GeV. Neutron flux densities at these high energies are calculated with codes like HETC or LAHET, the neutron cross sections are calculated in the codes from nuclear models. Below 20 MeV evaluated data files are applied together with transport codes like TWODANT or MCNP. Since several years work is in progress at different laboratories in order to extend the upper energy boundary of evaluated nuclear data to energies above 20 MeV, e.g. to 50 MeV, 150 MeV, 300 MeV.
In the following we describe the generation of a group constant set for the energy range from 10^{-5} to 50 MeV and its application in transport calculations. The work has been carried out in cooperation with the Obninsk Institute of Nuclear Engineering (INPE). INPE contributed the evaluated nuclear data in ENDF-6 format, the generation of the group constant library, test and application have been carried out at FZK.

Generation of a 75 group constant set in the energy range from 10^{-5} eV to 50 MeV

The evaluation of the nuclear data files up to 50 MeV has been carried by the Institute of Nuclear Power Engineering (INPE), Obninsk [1, 2].**Above 20 MeV** these cross sections have been obtained from nuclear model calculations and from available experimental data. Most of the data **below 20 MeV** have been adopted from evaluated nuclear data libraries (ENDF/B-VI, JENDL3.2). The data for $10^{-5}eV \leq E \leq 50MeV$ have been made available in ENDF-6 format. Cross sections of the following isotopes are included in our investigations: O^{16}, Pb^{208}, Th^{232}, Pa^{233}, U^{233}, U^{238}, Pu^{239} and Pu^{240} up to 50 MeV, and U^{235} (up to 300 MeV). Data for Fe^{56} and Cr^{52} which have been evaluated at INPE for the IFMIF project have been made available to us and are used in our calculations.

The nuclear data processing code NJOY [6] version 94.105 has been applied for the generation of the group constants. The 75 energy group structure is that of the 69 group WIMS set extended by 6 energy groups up to 50 MeV. The additional group boundaries are: 13.8, 15.0, 20.0, 27.1, 36.8 and 50.0 MeV. The group constants have been calculated for six temperatures: 300, 900, 1200, 1500, 2100 and 3000 K and for the seven values of the background cross section σ_0 : 10^{-3}, 10, 100, 1000, 10^4, 10^5, 10^{10} barn. Neutron transfer matrices are given until Legendre order P_5.

The group cross sections in 75 energy groups have been transformed to the Karlsruhe GRUBA format [7] which is the standard group constant format in the KArlsruhe PRogram System KAPROS [8] and can also be used with the deterministic transport code TWODANT [3]. By its secondary input option the GRUBA format allows easy change of group constants for selected isotopes, selected reaction types and for selected energy groups and therefore is a very useful tool for cross section testing.

Tests of the new 75 group constant library and its steering file

The GRUBA library and its steering file had to be modified to take into account reactions typical for energies above 10 MeV as e.g. (n,4n), $(n,2n+\alpha)$, $(n,3n+\alpha)$, $(n,2n+p)$, $(n,3np)$, $(n,2p)$, (n,pd). A new data type (MT=201) has been used on the Obninsk files: the energy angle distributions for continuum inelastic scattering and all threshold reactions with neutrons in the exit channel (e.g. (n,2n),(n,3n), (n,4n), (n,n+p), $(n,2n+\alpha)$.... are given as sum over all reactions; not included are discrete inelastic scattering and fission (MT=3,MF=18). Consequently neutron transfer matrices are calculated for elastic scattering, discrete inelastic scattering and for the sum of continuum inelastic scattering, (n,2n), (n,3n), (n,4n), $(n,2n+\alpha)$, ... The steering file for the new group constant set had to be modified accordingly.

These modifications have been intensively tested. As a typical test case a Pb^{208}- cylinder has been used with density and geometry corresponding to the lead target in the ADS Neutronic Benchmark [9] (radius: 10 cm, height: 50 cm). In the model that we used for our calculations a spatially homogeneous neutron source within a cylinder of radius 5 cm and height 10 cm in the center of the target was assumed. The energy dependence of the external source is similar to the one given in the Benchmark specification. The highest neutron energy of the external neutron source (source 1) is 10 MeV, the lowest energy is 111 keV. Comparisons have been carried out for results obtained from calculations with TWODANT in S_{16}/P_3 approximation with the 69 group constant library that has been used for the Benchmark calculations [9] and with the new 75 group constants. Comparisons for total neutron leakage, the neutron flux density and for different reaction rates are shown in Table 1. The first 2 columns of Table 1 show calculations for Pb^{208}. Pb^{208} data from INPE, Obninsk are based on ENDF/B-VI below 20 MeV. In order to eliminate from the comparison differences in nuclear data new Pb^{208} group constants in the 69 energy group structure have been calculated from ENDF/B-VI. The deviations of the results obtained with the old and with the new group constant set (relative to the results obtained with the old (69 group) set) are less than 1% except for a large deviation in the (n,α) reaction rate which is due to different data on ENDF/B-VI and on the Obninsk library.

Columns 4 and 5 show calculations with the 75 group set. The energy of the external source neutrons (source 2) is between 50 MeV and 111 keV. Neutron flux density and reaction rates are given for two coarse energy groups: coarse group 1 between 10 MeV and 50 MeV and coarse group 2 between 10^{-5} MeV and 10 MeV. The contribution of neutrons above 10 MeV to the total neutron flux is about 6 %. The contribution of neutrons above 10 MeV to the total reaction rate, the reaction rates for (n,γ), elastic and inelastic scattering is around 5 %. The contribution of neutrons above 10 MeV to the (n,2n) rate is about 93 % . For other threshold reactions ((n,3n), (n,p), (n,2p),.....) the contribution of neutrons above 10 MeV is more than 99 %.

Column 3 of Table 1 shows, that the capture reaction rate of Pb^{208} in the spectrum of the lead cylinder is only about 20 % of the capture reaction rate of Pb^{207}.

Application of the 75 group constant set for the calculation of k_{eff} and k_{source} of the ADS Neutronic Benchmark reactor

As a first application of the new 75 group constant set for a reactor we have recalculated the fresh core of the ADS Neutronic Benchmark [9]. The calculations have been carried out with TWODANT in S_8/P_3 approximation. Table 2 shows the results for k_{eff} and k_{source} for different U^{233} enrichment of the fuel.

The U^{233} enrichment that is necessary to obtain $k_{eff} = 0.96$ is lower (8.722 at %), when the new group constant set is applied. This is mainly due to the difference in the basic nuclear data below 10 MeV. On the Obninsk library the data for U^{233} and Th^{232} below 20 MeV are mainly from JENDL-3.2, most of the data for Pb^{208} below 20 MeV are are from ENDF/B-VI. In order to eliminate most of the differences in the data the cross sections for U^{233} and Th^{232} in the 69 group constant library were replaced by data from JENDL-3.2 and the cross sections of Pb^{208} were replaced by group constants obtained from ENDF/B-VI. In Table 2 the 69 group constant library with the replacements discussed above is called modified 69 group constant set.

The results for k_{eff} calculated with this modified 69 group constant set and with the 75 group constant set differ by about 1 % as is shown in Table 2. For k_{source} a similar difference is found.

Influence of different basic nuclear data for Th^{232} on k_{eff} of the ADS Neutronic Benchmark

In our original calculation for the ADS Neutronic Benchmark we used a 69 group constant set developed at FZK and mainly based on JEF-2.2. In further studies we found a remarkable change in k_{eff} of the ADS Neutronic Benchmark, when data for Th^{232} from other nuclear data libraries were used. In the calculations shown in Table 3 the 69 group constant set is used for the basic calculation (case 1). In additional calculations (case 2, 3, 4) the group constants for Th^{232} are replaced by group constants calculated from other nuclear data libraries, all other group constants are left unchanged. In case 2 the Th^{232} data are taken from ENDF/B-VI, k_{eff} is increased by 2.7 %, with Th^{232} group constants calculated from JENDL3.2 the increase is even larger, namely 4.6 % (case 3). Finally in case 4 only the (n,γ) cross section of Th^{232} was replaced from JENDL-3.2. As seen from the table k_{eff} is 4.3% larger than in the calculation with the unchanged group constant set (case 1).

The influence of the (n,γ) cross sections of Th^{232} has also been investigated in calculations with 75 energy groups. The group constants for the (n,γ) reaction were replaced by data from ENDF/B-VI in all energy groups below 20 MeV. This reduced k_{eff} by 1.6 % from 1.02431367 to 1.00795309.

Table 1 : Lead Target with external source
TWODANT calculations in S_8/P_3 approximation
comparison of neutron flux densities and reaction rates as a test
of the 75 group gruba library and the steering file

case	75 groups source 1 Pb^{208}	69 groups source 1 Pb^{208}	69 groups source 1 Pb^{207}	75 groups source 2 Pb^{208}	
	$E \leq 10MeV$			$E \leq$ 10MeV	$E \geq$ 10MeV
net leakage	1.016E+0	1.016E+0	1.021E+0	1.195E+0	1.195E+0
neutron flux	2.131E+1	2.119E+1	2.240E+1	2.281E+1	1.523E+0
reaction rates					
total	3.873E+0	3.865E+0	4.342E+0	4.142E+0	2.478E-1
capture	4.236E-4	4.217E-4	1.850E-3	4.332E-4	7.601E-4
(n,γ)	4.232E-4			4.330E-4	1.475E-5
(n,α)	4.147E-7	1.512E-6		1.973E-7	2.042E-4
(n, p)	4.978E-8	4.969E-8		8.350E-9	4.987E-4
(n, 2p)					4.789E-5
(n, p d)					1.053E-5
elastic	3.648E+0	3.637E+0	3.961E+0	3.999E+0	1.414E-1
inelastic	2.098E-1	2.111E-1	3.564E-1	1.400E-1	1.017E-2
(n,2n)	1.643E-2	1.641E-2	2.292E-2	2.594E-3	3.618E-2
(n,3n)	0.0	0.0	0.0	0.0	2.393E-2
(n,4n)	0.0	0.0	0.0	0.0	2.156E-2

Table 2: ADS Neutronic Benchmark

k_{eff} and k_{source} calculated with different group constant libraries

A. critiality calculations

U^{233} enrichment	k_{eff} 75 energy groups from Obninsk data (0-50 MeV)	69 energy groups modified set (0-10 MeV)
9.68	1.0243136	1.01362481
8.7216	.96000698	.94995146

B. source calculations

U^{233} enrichment atom percent	k_{source} 75 energy groups source up to 50MeV	69 energy groups modified set source up to 10 MeV
8.7216	.97643827$^{(1)}$ .97158054$^{(2)}$	.96300135

$$k_{source}^{(1)} = \frac{R(\nu \cdot fiss)+R(n,2n)+R(n,2n+x)+2\cdot[R(n,3n)+R(n,3n+x)]+3R(n,4n)}{L+R(abs)}$$

$$k_{source}^{(2)} = \frac{R(\nu \cdot fiss)+R(n,2n)}{L+R(abs)}$$

R: reaction rate

(n,2n+x): (n,2n + p) + $(n,2n+\alpha)$ + $(n,2n+2\alpha)$

(n,3n+x): (n,3n + p) + $(n,3n+\alpha)$

L: net leakage

Table 3 : ADS Neutronic Benchmark **Influence of different nuclear data for Th^{232} on k_{eff}** **TWODANT calculations in S_8/P_3 approximation**				
data base for Th^{232}	FZKG69-set (Th^{232} from JEF-2.2) (case 1)	Th^{232} from ENDF/B-VI (case 2)	Th^{232} from JENDL-3.2 (case 3)	only $\sigma(n,\gamma)$ for Th^{232} from JENDL-3.2 (case 4)
k_{eff}	.96142897	.98713736	1.00546073	1.00271764
$(k_{eff} - k_{eff,1})/k_{eff,1}$	$(k_{eff,1})$	2.7 %	4.6 %	4.3 %

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