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Validation of computer code TORT, (with BUGLE-7 and BUGLE-96 libraries) using RC Rez Iron Spherical Assemblies producing neutron and gamma mixed fields

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May 12, 2020.

Introduction

- Validation of the TORT computing program with the BUGLE-B7 library was performed by comparing the calculation and measurement of leakage neutron and gamma spectra on pure iron spherical assemblies.

- Five sets of Fe spherical geometry were selected,

20, 30, 40, 50 and 100 cm diameter iron spheres with a Cf-252 neutron source located in the center of the Fe sphere.

Evaluated measured spectra (neutrons and gamma) were obtained from **L.A. Trykov (FEI Obninsk).** Spectra were measured in RC Rez, only Fe sphere of diameter 40cm was measured in Obninsk.

We suppose that this access enables the obtaining **consistent results from one author** [4].

Neutron spectra measurements were carried out by the proton recoil method (stilbene and proportional hydrogen detector), and gamma spectra were measured with stilbene.

Calculation using code TORT

- The calculation (with a constant neutron source) was performed by the transport 3D program TORT [2,3], solving the Boltzmann transport equation in **$S_N P_L$ approximation** in **cylindrical equidistant coordinates R-Theta-Z**. The set of directions S8 used represents 96 discrete directions. The development according to Legendre polynomials up to the 3rd order (P3) was used in the calculation.
- The step of the **R-Theta-Z** computer network was **0.5 cm - 4.5 ° - 0.5 cm**.
  The BUGLE-96 and BUGLE-B7 nuclear data libraries (derived from the ENDF / B-VI and ENDF / B-VII libraries, respectively) were used for the calculation.

Fig.1 Principal scheme of leakage neutron spectra measurement

Principal scheme of the leakage neutron spectrum measurement

Iron sphere of diam. 100cm.

Shadow Cone:
Fe – iron,
PE+B
(polyethylene
with boron)

Other assemblies are simmilar

EFFECT E EVALUATION
A = E + AB + FB + LB - meas. without shadow cone
B = AB + FB + LB - meas. with shadow cone
E = A - B

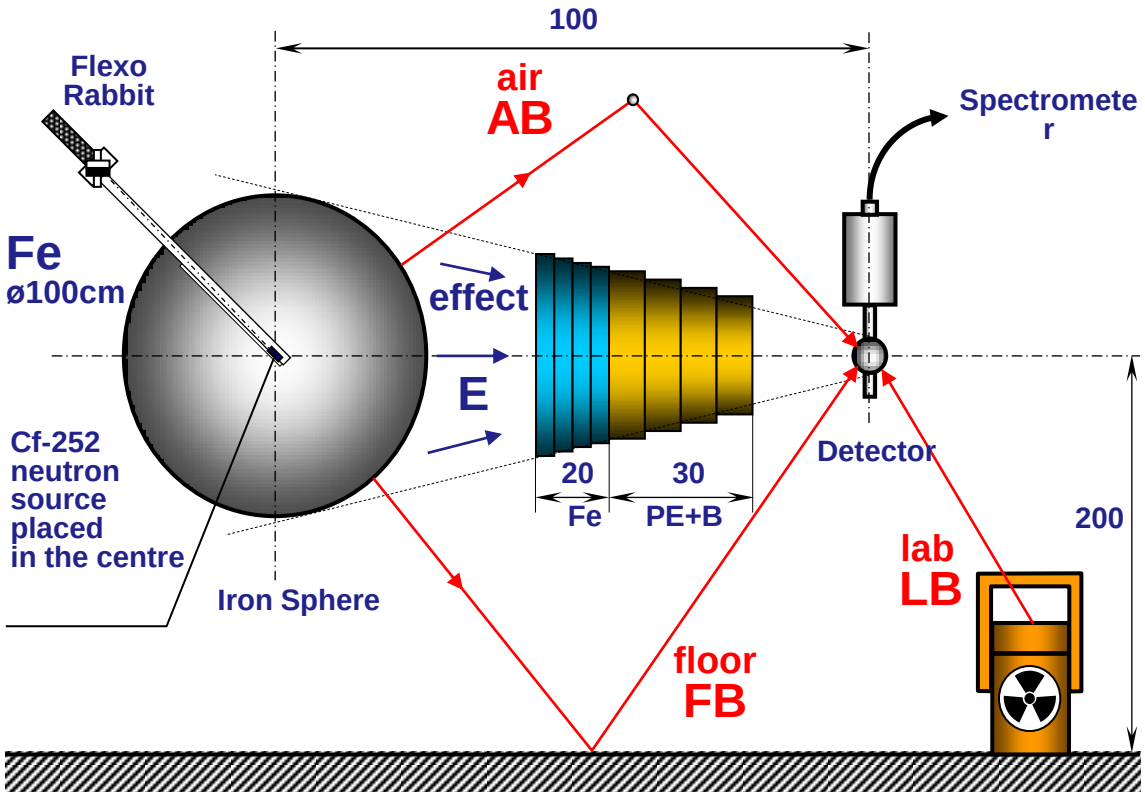


Fig.2 Shielding cones for gamma and neutrons

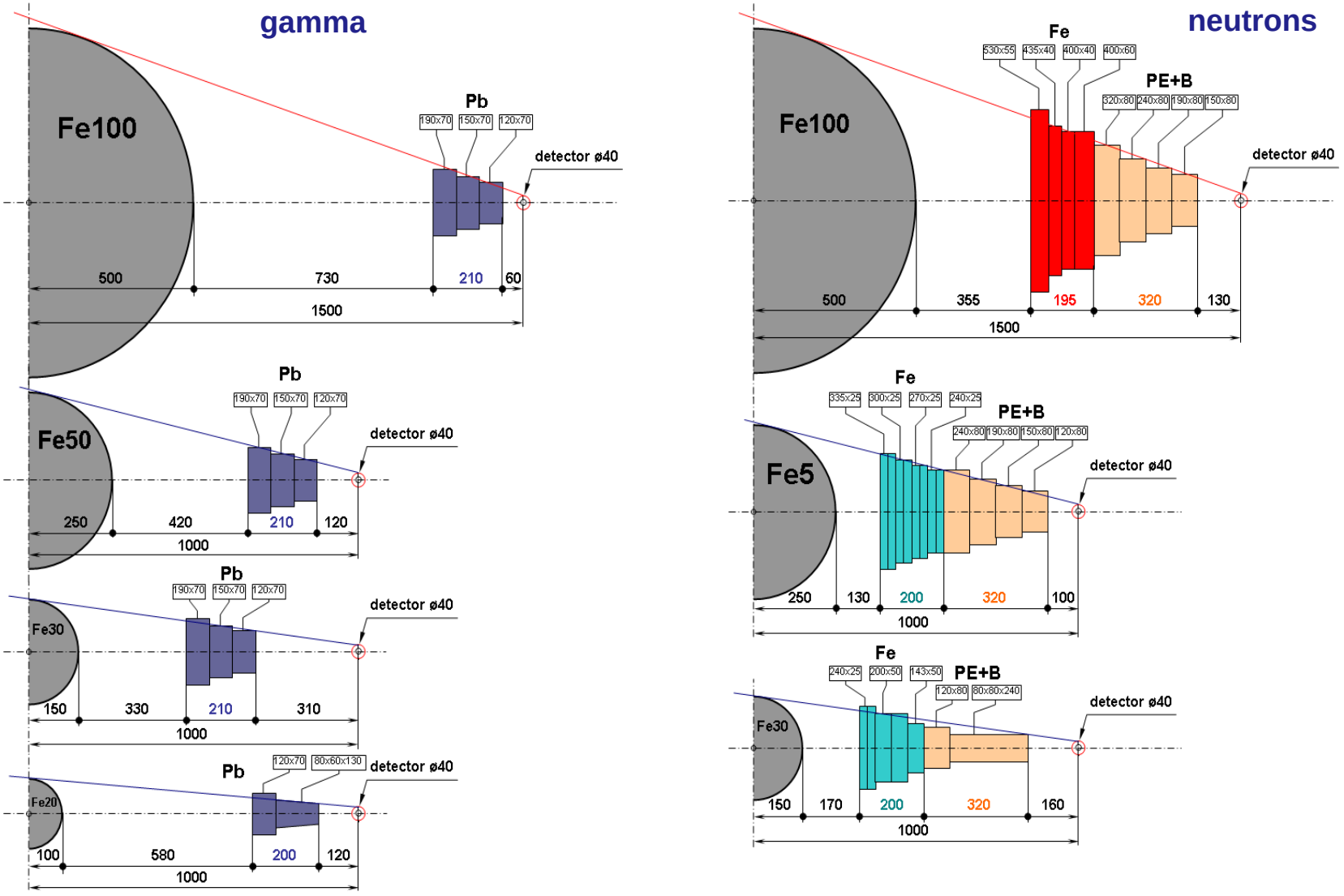


Fig.3 TORT model of benchmark assembly FE DIA50, R100

- Drawing is in scale
- **R-Theta-Z** computer network was **0.5cm - 4.5 ° - 0.5cm**.

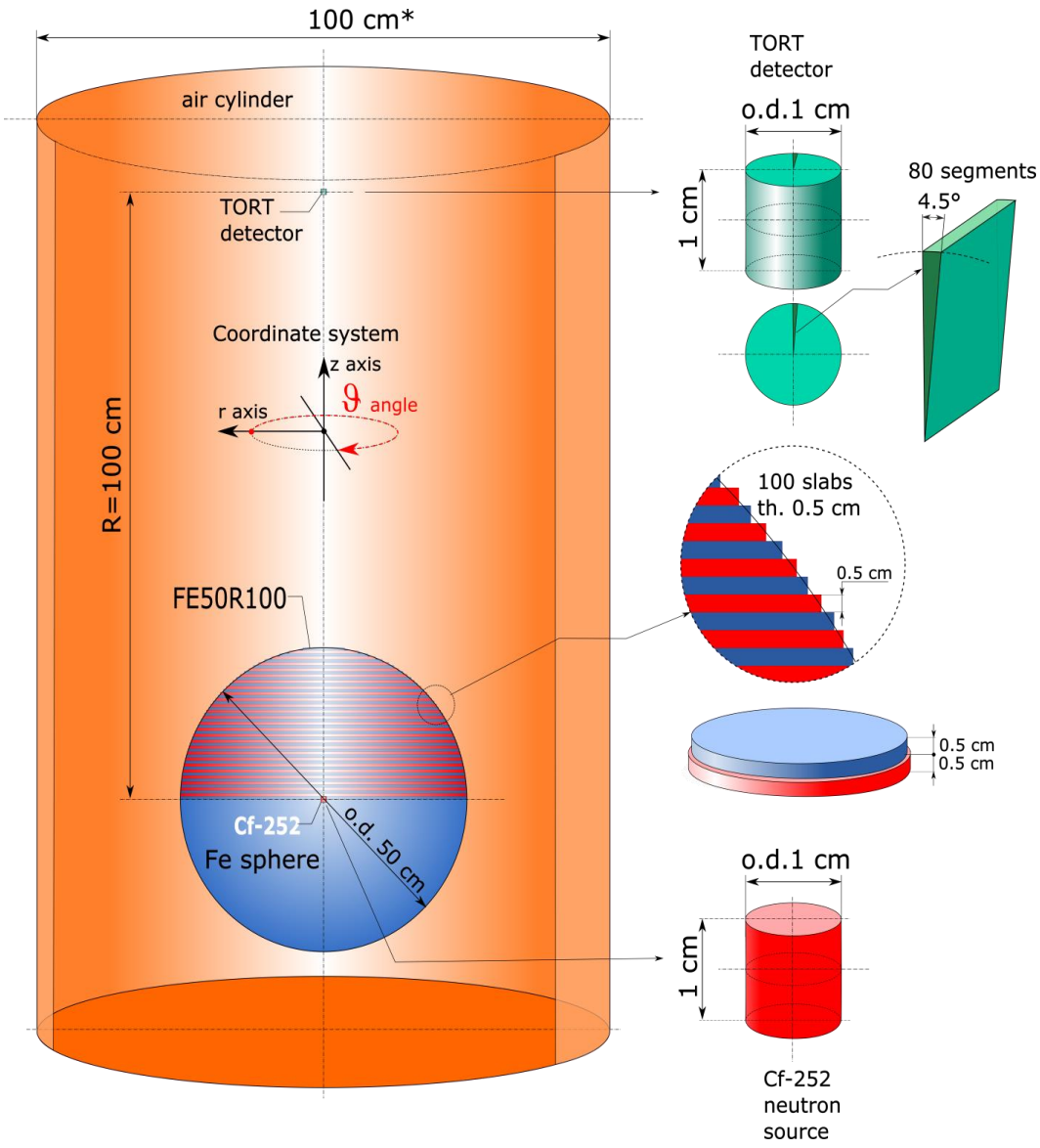
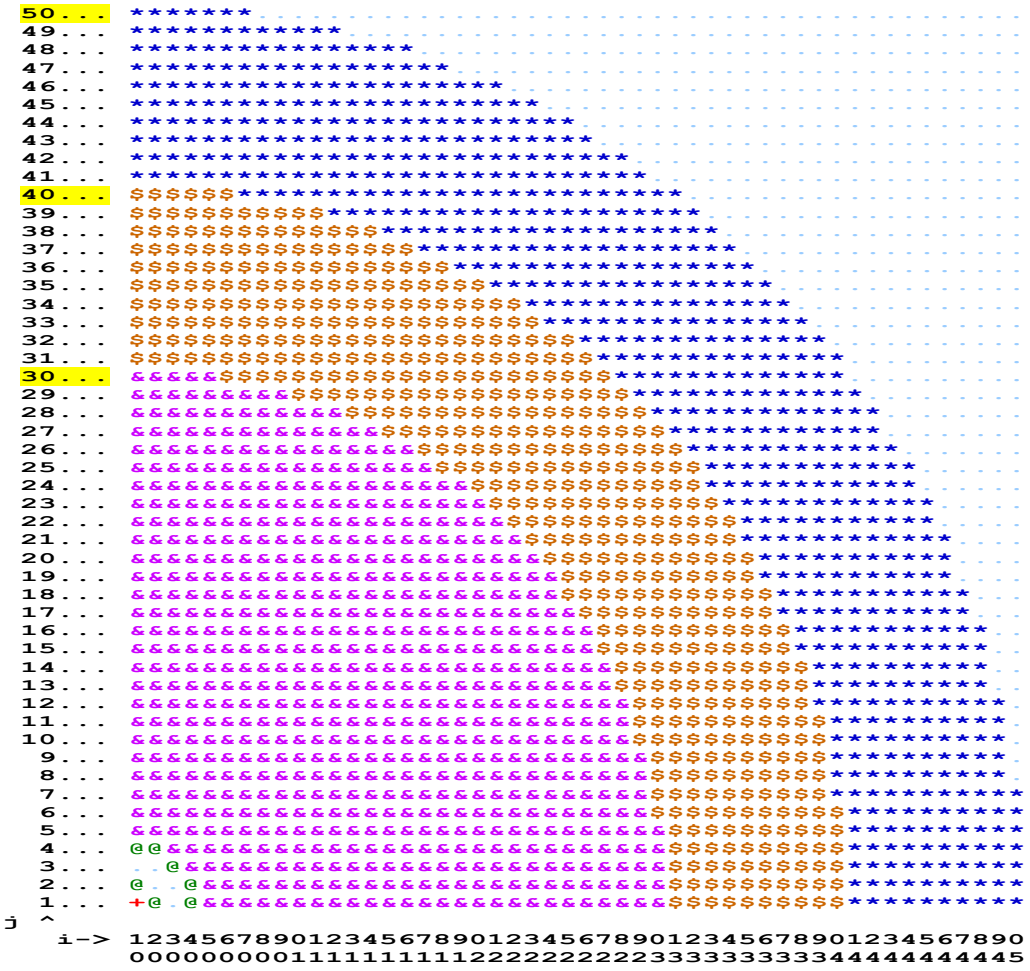


Fig.4, Program TORT, model of Fe sphere of diameter 30,40,50 cm (step 0.5cm)



Obr. 2 Výpočet programem TORT, schéma modelování Fe-koule o průměru 30, 40 a 50cm. Fe disky výšce 0,5cm s měnícím se průměrem a jsou naskládány do vnitřního objemu dané koule.

Adjustment of TORT calculated results to experimental data

- As part of the analysis of the TORT results, it was found that the total integral of the spectrum I (0.01 - 20MeV) does not correspond to the completely expected values for some Fe spheres, see Tab.1see Tab.1 column V2 TORT.

- The usual value of the that integral depending on the thickness of Fe is presented in column 3 (Trykov, exp) and column 4 (Blokhin, calculation,JEFF-3.3). The correction adjustment (Multiplication factor for TORT) was determined using the results of the Blokhin calculation, see tab.1.
- **Comment:**
- The calculation of Fe spheres using TORT was performed in the laboratory for the first time in two stages. The results of both stages are not completely consistent, therefore **further methodological calculations are planned (eg use a finer step, etc.)**

Tab.1, Determination of the multiplication correction factors for TORT results.

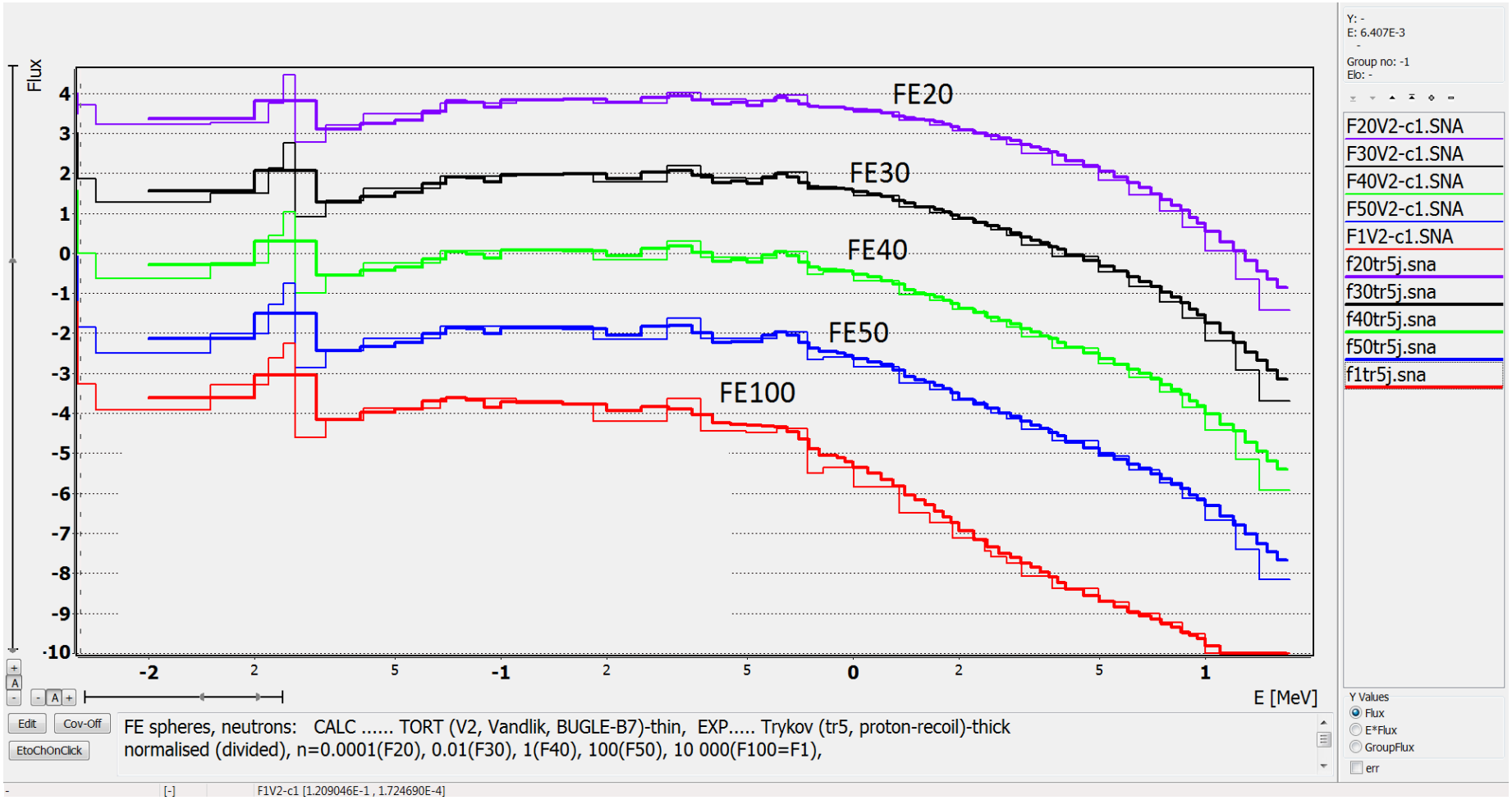
Tab T, Determination of the multiplication correction factor for TORT

	n-spectrum integral, En (0.01-10MeV) [1]				
Assembly	V2-TORT CALC Buggle-B7	Trykov EXP	Blochin MCNP CALC JEFF-3.3	V2-CALC, corrected integral	Corr.Factor Blochin/V2 (multiplying)
FE DIA 20	0.8940	0.984	0.9949	0.9949	1.11286
FE DIA 30	0.9870	0.962	0.9916	0.9916	1.00466
FE DIA 40	1.0112	0.974	0.9872	0.9872	0.97627
FE DIA 50	1.0260	0.954	0.9828	0.9828	0.95789
FE DIA 100	0.7370	0.838	0.8654	0.8654	1.17422

note: I40=(I30+I50) /2

0.9872

Fig.5 Results C/E-neutrons , EXP=thick (proper normalisation used)



Tab. 2 Results C/E- neutrons, overview for all Fe thicknesses .

Tab. neutrons -overview

En range[MeV]		FE20	FE30	FE40	FE50	FE100	Trend in C/E with
from	to	C/E	C/E	C/E	C/E	C/E	**increasing Fe thickness**
0.01	17.00	1.010	1.030	1.013	1.030	1.033	total
0.01	0.03	1.030	1.135	1.273	1.370	1.802	increasing (24keV region)
0.03	0.10	1.077	1.133	1.190	1.197	1.058	
0.10	0.20	0.955	0.962	0.962	1.011	0.893	const., **C/E agreement,**
0.20	0.40	1.039	1.021	1.008	1.061	0.980	const., **C/E agreement,**
0.40	0.80	1.232	1.198	1.125	1.086	0.805	decreasing
0.80	1.00	0.995	0.947	0.874	0.790	0.535	decreasing
1.00	2.00	0.931	0.920	0.846	0.766	0.470	decreasing
2.00	3.00	0.892	0.910	0.933	0.948	0.728	*const., **C/E agreement,**
3.00	5.00	0.739	0.824	0.843	0.888	0.779	*increasing
5.00	7.00	0.678	0.789	0.838	0.986	1.096	increasing
7.00	10.00	0.679	0.739	0.805	0.972	1.202	increasing
10.00	17.00	0.391	0.413	0.442	0.501	0.655	increasing

0.95<C/E<1.05	* except FE 100
1.05<C/E<1.10	
C/E>1.10	
0.9<C/E<0.95	
C/E<0.9	

Conclusions to neutrons, see. Table2

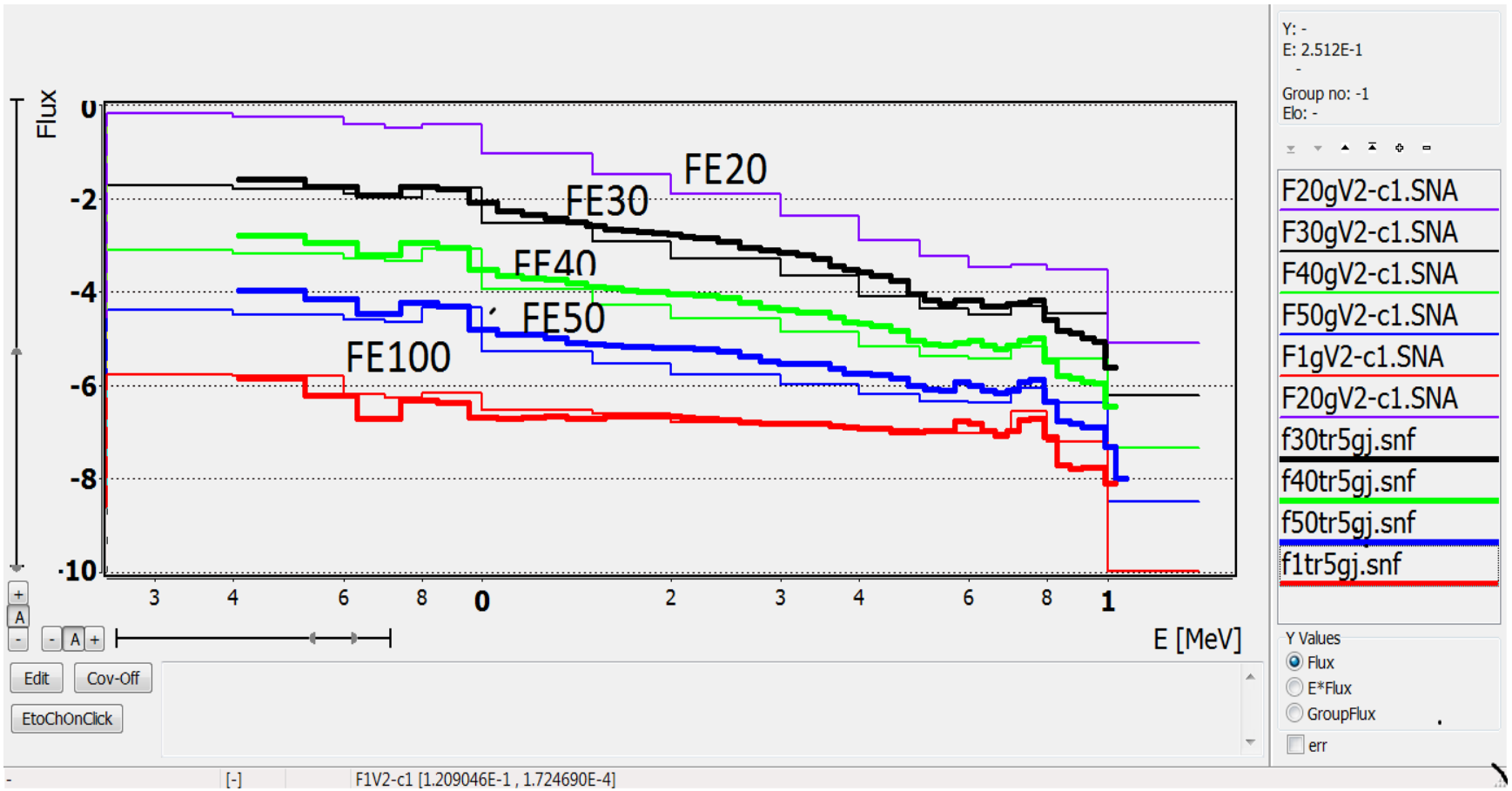
1) The TORT results for neutron are in **better agreement then for gamma**.
the same conclusion applies to MCNP calculations

2) Tab. 2, It is possible to observe **clear trends wit Fe slab increasing**

3) Tab.2, **Good agreement in region 0.1-0.4MeV and 2-3 MeV region**

4) Needed further methodological TORT calculations (eg use a finer step, etc.), to explain Why integral I(0.01-10MeV>1 etc.

Fig.6 Results C/E- gamma, EXP=thick (proper normalisation used),FE20-only calc



Tab. 3 Results C/E-gamma, overview for all Fe thicknesses.

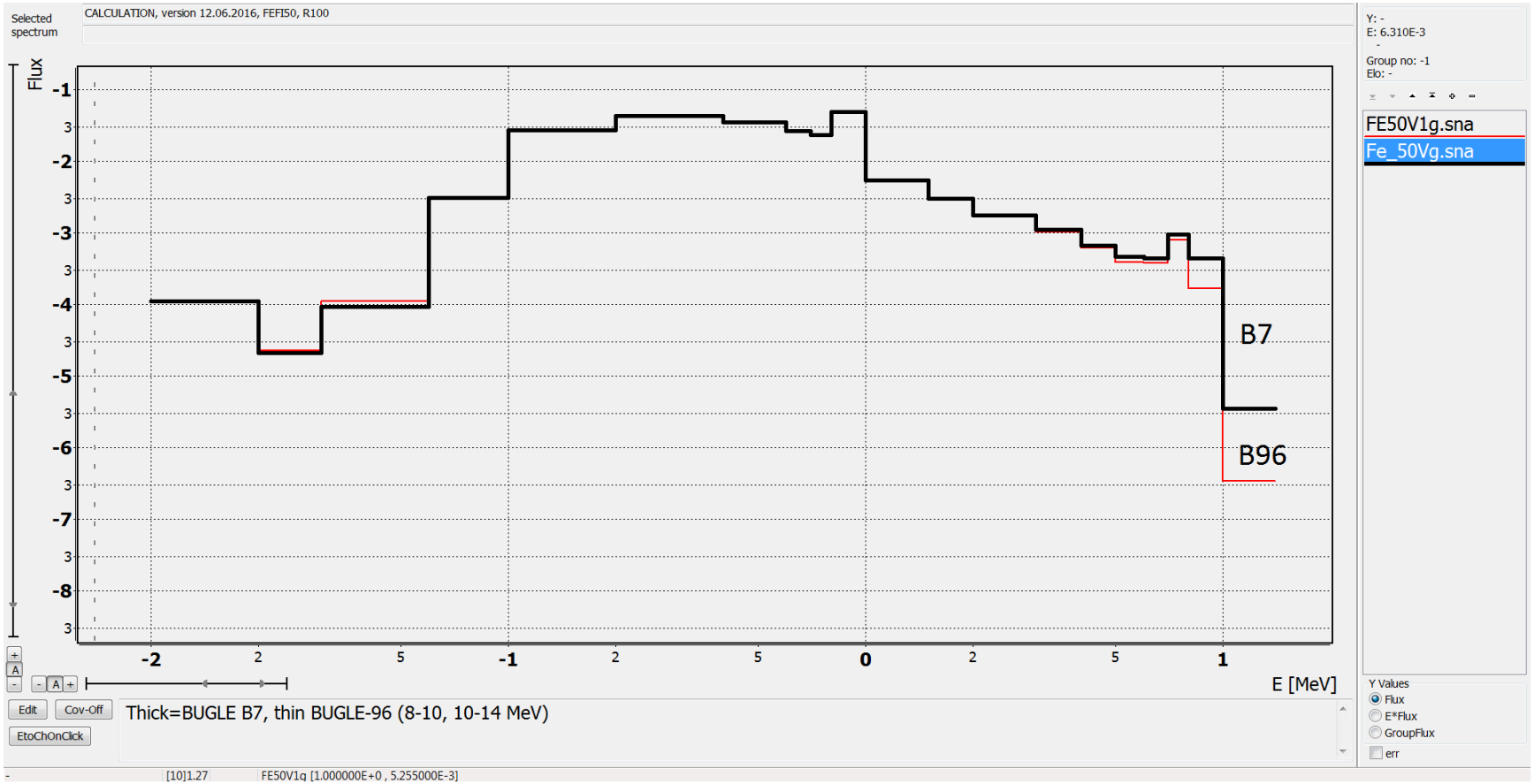
Tab. gamma -overview

Eg range[MeV]		FE30	FE40	FE50	FE100		Trend in C/E with increasing
from	to	CLC/EXP	CLC/EXP	CLC/EXP	CLC/EXP	Characteristics of region	Fe thickness
0.407	10.000	0.756	0.605	0.532	1.276	**total** integral	*decreasing
0.407	0.700	0.748	0.504	0.395	1.580	**511keV** region of annihilation peak	*decreasing
0.700	1.000	0.985	0.861	0.846	1.676	**847keV**, Fe-56, inelastic scatter. peak	*decreasing (sllightly)
1.000	5.500	0.560	0.476	0.415	1.063	not big peaks region	*decreasing
5.500	6.500	0.647	0.492	0.457	0.677	**5.9 and 6 MeV**, Fe-56 n-capture	*decreasing
6.500	8.500	0.871	0.794	0.814	1.502	**7.6 MeV**, Fe-56 n-capture, dominant peak	*nearly constant
8.500	10.000	3.156	3.054	3.100	3.659	**9.3MeV**, Fe-54; n-capture	*constant

	0.90<C/E<1.10
	1.10<C/E<1.20
	C/E>1.20
	0.80<C/E<0.90
	C/E<0.80

* except FE 100

Fig.7, FE DIA50, R100,gamma,Calc.TORT , BUGLE-B7 thick, BUGLE-96 thin



Conclusions to gamma, see. Table 3

- 1) BUGLE-7 and BUGLE-96 library,
  B7, wrong results in groups (8-10, MeV) with linie 9.3 MeV
  (Fe-54…n-capture), and 10-14 MeV, fig.7
  perhaps wrong isotopic composition for Fe-54? See Tab.3
- 2) good agreement for main Fe linien
  847 keV…..Fe-56 inelastic
  7635 keV….Fe-56 …n capture
  (background not subracted)

References

1) B. Janský, E. Novák, P. Otopal, *Data for Calculation of Neutron and Gamma Leakage Spectra from Iron and Water Spheres with Cf-252 Neutron Source in Centre* , Report NRI, ÚJV 11506, Řež (2000).

2) W. A. Rhoades. F. R. Mynatt. *The TORT/PC Three-Dimensional Discrete Ordinate Neutron/Photon Transport Code. CCC-543*. RSIC. March 1994

3) DLC-0245/002: *VITAMIN-B7/BUGLE-B7. Broad-Group and Fine-Group and Coupled Neutron/Gamma Cross-Section Libraries.* Most Recent Update: August 2012

4) L.A.Trykov et all, *Integral experiments in ionizing radiation transport problems*, Energoatomizdat, Moscow 1985

5) Jánský B., Novák E.,Turzík Z.,Otopal P., Čuda P., *Technický Návrh Referenčních Směsných Polí Neutronů A Gama*, zpráva ÚJV 11700-R,D, Řež 2001

Attachment: FE DIA20, R100-neutrons

Tab.( )FE20N- Assemby FE DIA 20, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.01	17.00	9.85E-01	1.15	9.95E-01	0	1.010E+00	1.15
0.01	0.03	8.64E-03	7.78	8.90E-03	0	1.030E+00	7.78
0.03	0.10	2.54E-02	4.24	2.74E-02	0	1.077E+00	4.24
0.10	0.20	6.96E-02	7.07	6.65E-02	0	9.547E-01	7.07
0.20	0.40	1.44E-01	4.76	1.50E-01	0	1.039E+00	4.76
0.40	0.80	2.34E-01	2.04	2.88E-01	0	1.232E+00	2.04
0.80	1.00	8.65E-02	2.50	8.61E-02	0	9.953E-01	2.50
1.00	2.00	2.51E-01	1.65	2.33E-01	0	9.313E-01	1.65
2.00	3.00	8.92E-02	2.92	7.95E-02	0	8.922E-01	2.92
3.00	5.00	5.70E-02	2.74	4.21E-02	0	7.388E-01	2.74
5.00	7.00	1.45E-02	4.78	9.85E-03	0	6.775E-01	4.78
7.00	10.00	4.62E-03	4.65	3.14E-03	0	6.793E-01	4.65
10.00	17.00	7.98E-04	5.32	3.12E-04	0	3.911E-01	5.32

	0.95<C/E<1.05
	1.05<C/E<1.10
	C/E>1.10
	0.9<C/E<0.95
	C/E<0.9

Attachment: FE DIA30, R100-neutrons

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Tab.( )FE30N- Assemby FE DIA 30, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.01	17.00	9.62E-01	1.39	9.92E-01	0	1.030E+00	1.39
0.01	0.03	1.52E-02	7.99	1.72E-02	0	1.135E+00	7.99
0.03	0.10	3.51E-02	4.15	3.98E-02	0	1.133E+00	4.15
0.10	0.20	9.40E-02	7.07	9.03E-02	0	9.616E-01	7.07
0.20	0.40	1.91E-01	4.79	1.95E-01	0	1.021E+00	4.79
0.40	0.80	2.68E-01	2.04	3.22E-01	0	1.198E+00	2.04
0.80	1.00	8.33E-02	2.50	7.88E-02	0	9.470E-01	2.50
1.00	2.00	1.90E-01	1.73	1.74E-01	0	9.201E-01	1.73
2.00	3.00	5.07E-02	2.93	4.61E-02	0	9.095E-01	2.93
3.00	5.00	2.63E-02	2.76	2.16E-02	0	8.242E-01	2.76
5.00	7.00	6.41E-03	4.76	5.06E-03	0	7.892E-01	4.76
7.00	10.00	2.26E-03	4.61	1.67E-03	0	7.393E-01	4.61
10.00	17.00	4.12E-04	5.30	1.70E-04	0	4.126E-01	5.30

	0.95<C/E<1.05
	1.05<C/E<1.10
	C/E>1.10
	0.9<C/E<0.95
	C/E<0.9

Attachment: FE DIA40, R100-neutrons

Tab.( )FE40N- Assemby FE DIA 40, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.01	17.00	9.74E-01	1.62	9.87E-01	0	1.013E+00	1.62
0.01	0.03	2.51E-02	8.17	3.19E-02	0	1.273E+00	8.17
0.03	0.10	4.59E-02	4.11	5.46E-02	0	1.190E+00	4.11
0.10	0.20	1.18E-01	7.07	1.13E-01	0	9.618E-01	7.07
0.20	0.40	2.33E-01	4.85	2.34E-01	0	1.008E+00	4.85
0.40	0.80	2.90E-01	2.05	3.26E-01	0	1.125E+00	2.05
0.80	1.00	7.52E-02	2.50	6.57E-02	0	8.740E-01	2.50
1.00	2.00	1.43E-01	1.81	1.21E-01	0	8.461E-01	1.81
2.00	3.00	2.74E-02	2.94	2.55E-02	0	9.325E-01	2.94
3.00	5.00	1.30E-02	2.77	1.09E-02	0	8.430E-01	2.77
5.00	7.00	3.10E-03	4.75	2.60E-03	0	8.382E-01	4.75
7.00	10.00	1.13E-03	4.56	9.14E-04	0	8.053E-01	4.56
10.00	17.00	2.24E-04	5.23	9.90E-05	0	4.420E-01	5.23

	0.95<C/E<1.05
	1.05<C/E<1.10
	C/E>1.10
	0.9<C/E<0.95
	C/E<0.9

Attachment: FE DIA50, R100-neutrons

Tab.( )FE50N- Assemby FE DIA 50, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.01	17.00	9.55E-01	1.80	9.83E-01	0	1.030E+00	1.80
0.01	0.03	3.93E-02	8.32	5.38E-02	0	1.370E+00	8.32
0.03	0.10	5.99E-02	4.11	7.17E-02	0	1.197E+00	4.11
0.10	0.20	1.33E-01	7.07	1.34E-01	0	1.011E+00	7.07
0.20	0.40	2.49E-01	4.91	2.64E-01	0	1.061E+00	4.91
0.40	0.80	2.84E-01	2.05	3.08E-01	0	1.086E+00	2.05
0.80	1.00	6.43E-02	2.51	5.08E-02	0	7.901E-01	2.51
1.00	2.00	1.04E-01	1.88	7.95E-02	0	7.663E-01	1.88
2.00	3.00	1.42E-02	2.94	1.35E-02	0	9.477E-01	2.94
3.00	5.00	5.96E-03	2.78	5.29E-03	0	8.877E-01	2.78
5.00	7.00	1.29E-03	4.75	1.28E-03	0	9.861E-01	4.75
7.00	10.00	4.91E-04	4.54	4.78E-04	0	9.723E-01	4.54
10.00	17.00	1.12E-04	5.25	5.58E-05	0	5.005E-01	5.25

	0.95<C/E<1.05
	1.05<C/E<1.10
	C/E>1.10
	0.9<C/E<0.95
	C/E<0.9

Attachment: FE DIA100, R150-neutrons

Tab.( )FE100N- Assemby FE DIA 100, R150, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.01	17.00	8.38E-01	3.69	8.65E-01	0	1.033E+00	3.69
0.01	0.03	1.14E-01	12.18	2.05E-01	0	1.802E+00	12.18
0.03	0.10	1.11E-01	6.05	1.17E-01	0	1.058E+00	6.05
0.10	0.20	1.80E-01	10.64	1.61E-01	0	8.932E-01	10.64
0.20	0.40	2.42E-01	7.36	2.37E-01	0	9.800E-01	7.36
0.40	0.80	1.61E-01	3.58	1.29E-01	0	8.050E-01	3.58
0.80	1.00	1.58E-02	3.54	8.46E-03	0	5.352E-01	3.54
1.00	2.00	1.42E-02	3.05	6.66E-03	0	4.699E-01	3.05
2.00	3.00	5.66E-04	4.53	4.12E-04	0	7.277E-01	4.53
3.00	5.00	1.47E-04	4.46	1.15E-04	0	7.790E-01	4.46
5.00	7.00	2.70E-05	7.13	2.96E-05	0	1.096E+00	7.13
7.00	10.00	1.27E-05	6.56	1.52E-05	0	1.202E+00	6.56
10.00	17.00	4.09E-06	7.30	2.68E-06	0	6.547E-01	7.30

	0.95<C/E<1.05
	1.05<C/E<1.10
	C/E>1.10
	0.9<C/E<0.95
	C/E<0.9

Attachment: FE DIA20, R100-gamma, calculation TORT,(measurement is not available)

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Tab.( )FE20G- Assemby FE DIA 20, R100, m

Energy range[MeV]		Integral values	
from	to	EXP	U[%]
0.407	10.000	3.34E-01	0
0.407	0.700	1.47E-01	0
0.700	1.000	1.07E-01	0
1.000	5.500	7.83E-02	0
5.500	6.500	4.56E-04	0
6.500	8.500	6.82E-04	0
8.500	10.000	4.39E-04	0

Attachment: FE DIA30, R100-gamma

Tab.( )FE30G- Assemby FE DIA 30, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.407	10.000	1.56E-01	4.100	1.18E-01	0	7.560E-01	4.100
0.407	0.700	5.76E-02	9.490	4.30E-02	0	7.475E-01	9.490
0.700	1.000	4.46E-02	5.990	4.39E-02	0	9.850E-01	5.990
1.000	5.500	5.17E-02	2.410	2.90E-02	0	5.598E-01	2.410
5.500	6.500	6.00E-04	7.830	3.88E-04	0	6.473E-01	7.830
6.500	8.500	9.36E-04	6.500	8.15E-04	0	8.711E-01	6.500
8.500	10.000	1.59E-04	9.750	5.00E-04	0	3.156E+00	9.750

	0.90<C/E<1.10
	1.10<C/E<1.20
	C/E>1.20
	0.80<C/E<0.90
	C/E<0.80

Attachment: FE DIA40, R100-gamma

Tab.( )FE40G- Assemby FE DIA 40, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.407	10.000	8.92E-02	4.250	5.39E-02	0	6.045E-01	4.250
0.407	0.700	3.44E-02	9.670	1.73E-02	0	5.037E-01	9.670
0.700	1.000	2.50E-02	6.210	2.15E-02	0	8.607E-01	6.210
1.000	5.500	2.75E-02	2.230	1.31E-02	0	4.762E-01	2.230
5.500	6.500	7.99E-04	7.840	3.93E-04	0	4.918E-01	7.840
6.500	8.500	1.29E-03	6.710	1.03E-03	0	7.940E-01	6.710
8.500	10.000	1.84E-04	9.730	5.60E-04	0	3.054E+00	9.730

	0.90<C/E<1.10
	1.10<C/E<1.20
	C/E>1.20
	0.80<C/E<0.90
	C/E<0.80

Attachment: FE DIA50, R100-gamma

Tab.( )FE50G- Assemby FE DIA 50, R100, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.407	10.000	5.75E-02	4.270	3.06E-02	0	5.320E-01	4.270
0.407	0.700	2.26E-02	9.850	8.92E-03	0	3.949E-01	9.850
0.700	1.000	1.38E-02	6.200	1.17E-02	0	8.463E-01	6.200
1.000	5.500	1.84E-02	2.160	7.62E-03	0	4.151E-01	2.160
5.500	6.500	9.57E-04	7.960	4.38E-04	0	4.571E-01	7.960
6.500	8.500	1.62E-03	6.810	1.32E-03	0	8.136E-01	6.810
8.500	10.000	2.03E-04	9.690	6.29E-04	0	3.100E+00	9.690

	0.90<C/E<1.10
	1.10<C/E<1.20
	C/E>1.20
	0.80<C/E<0.90
	C/E<0.80

Attachment: FE DIA100, R150-gamma

Tab.( )FE100G- Assemby FE DIA 100, R150, measurement and calculation (TORT)

Energy range[MeV]		Integral values					
from	to	EXP	U[%]	CALC	U[%]	CALC/EXP	U[%]
0.407	10.000	1.45E-02	3.490	1.85E-02	0	1.276E+00	3.490
0.407	0.700	2.38E-03	14.440	3.76E-03	0	1.580E+00	14.440
0.700	1.000	1.13E-03	9.130	1.90E-03	0	1.676E+00	9.130
1.000	5.500	6.99E-03	3.260	7.44E-03	0	1.063E+00	3.260
5.500	6.500	1.39E-03	10.720	9.41E-04	0	6.770E-01	10.720
6.500	8.500	2.34E-03	9.200	3.51E-03	0	1.502E+00	9.200
8.500	10.000	2.60E-04	14.490	9.51E-04	0	3.659E+00	14.490

	0.90<C/E<1.10
	1.10<C/E<1.20
	C/E>1.20
	0.80<C/E<0.90
	C/E<0.80

TORT

- note:
- N=8,…..96 směrů (8x8+něco=směry v oddělujících rovinách)
- L=3….0 člen a dále koficienty u prvních 3 polynomů Lagr.