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Proposal for Subgroup 18 /Coordinator A.V.Ignatyuk/

**THORIUM COMPUTATIONAL BENCHMARKS**

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**Introduction**

Four fast critical assemblies were investigated in IPPE at the end of 80th for the validation of thorium neutron data. Each assembly has a central region consisted from heterogeneous mixture of thorium, high enriched uranium and polyethylene. These materials were included in stainless steel tubes and the heterogeneity structures were close to the lattices from flat layers. A composition of each lattice was adjusted so that k-infinity was close to unit. The criticality of whole assembly in every case was provided by surrounding the central region by a driver zone with much higher concentration of enriched uranium and than by a depleted uranium reflector. The dimensions of central regions in all cases were large enough and neutron spectra established in the centers of assemblies were close to those for the fundamental mode. So-called "zero reactivity" method was used for determination of k-infinity. The idea of a method is the measurement of the ratio of central cell reactivity to reactivity worth of U-235. If k-infinity is equal to unit this ratio is equal to zero. A small deviation of the ratio from zero can be simply expressed by the deviation of k-infinity from unit. Besides reactivity worth ratios and the determination of k-infinity some cross section rates were measured in the centers of assemblies.

The computational benchmark models proposed represent the simplified models of experimental lattices. We consider that these benchmarks as the first stage of international validation of thorium neutron data. On the next stage the comparison with experimental data should be considered.

**Benchmark models**

Each benchmark model represents a flat layer lattice. Four different layer materials were used:

1. Highly enriched (90%) uranium oxide;
2. Intermediate enriched (36%) uranium oxide;
3. Thorium metal;
4. Polyethylene.

Atomic densities for each materials are given in the Table 1. Compositions of materials correspond to the structural materials used in the experiments.

Lattice structures are shown on the Figs. 1 - 4. The dimensions of layers are indicated in the figure captures.

### What should be calculated?

For each benchmark the following parameters must be calculated:

1. k-infinity;
2. The cross sections averaged over the energy and over the cell with the weight of neutron flux for the reactions:

U-235 (n, fission); U-238 (n, fission); Th-232 (n, fission);

U-235 (n, capture); U-238 (n, capture); Th-232 (n, capture);

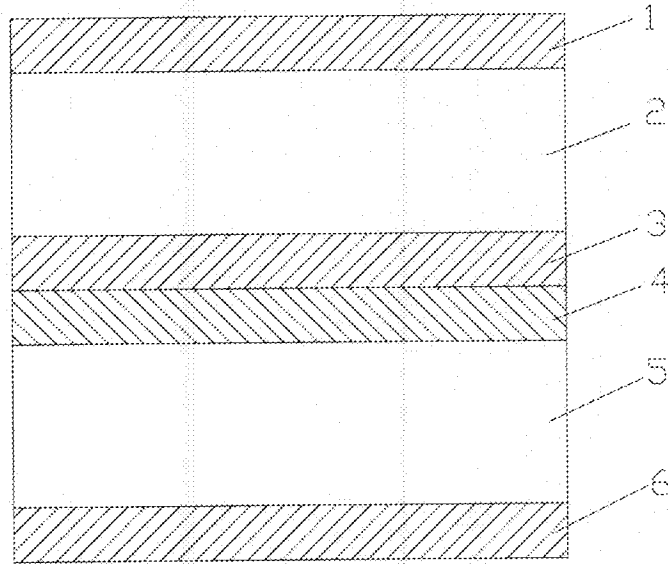
Fe (n, capture); Cr (n, capture); Ni (n, capture);

Au (n, capture).

3. Averaged over the cell both the fission and capture rates for each nuclides.

Table 1. Composition of layers

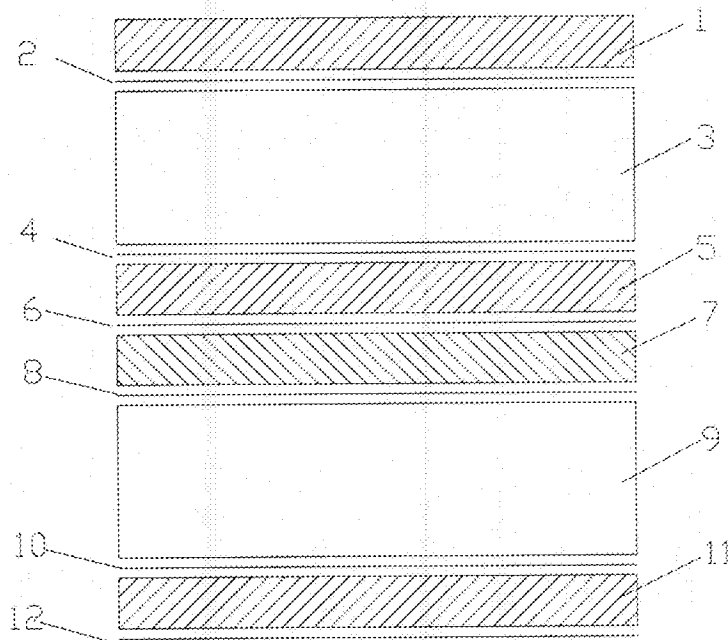
Layer Material	Highly enriched UO <sub>2</sub>	Interm. enriched UO <sub>2</sub>	Thorium	Polyethylene
U-235	0.00781	0.00334		
U-238	0.00085	0.00546		
Th-232			0.01972	
Oxygen	0.01751	0.01751		
Aluminum			0.00401	
Iron	0.01533	0.01533	0.00418	0.00418
Chromium	0.00423	0.00423	0.00113	0.00113
Nickel	0.00204	0.00204	0.00058	0.00058
Manganese	0.00031	0.00031	0.00007	0.00007
Carbon				0.02789
Hydrogen				0.05577



**Figure 1**

The unit cell # 1

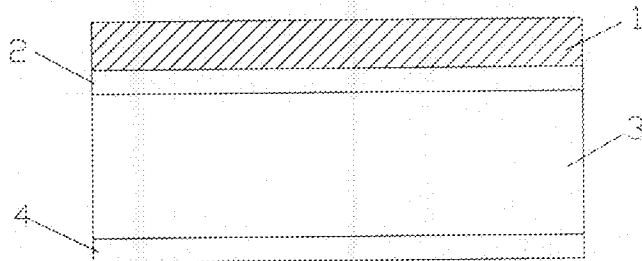
- 1, 3,6 -  $\text{UO}_2$  (90%),  $\Delta t = 0.173$  cm
- 4 -  $\text{UO}_2$  (36%),  $\Delta t = 0.173$  cm
- 2,5 - Th (met),  $\Delta t = 1.01$  cm



**Figure 2**

The unit cell # 2

- 1,5,11 -  $\text{UO}_2$  (90%),  $\Delta t = 0.173$  cm
- 7 -  $\text{UO}_2$  (36%),  $\Delta t = 0.173$  cm
- 3,9 - Th (met),  $\Delta t = 1.01$  cm
- 2,4,6,8,10,12- Polyethylene ( $\text{CH}_2$ ),  $\Delta t = 0.015$  cm



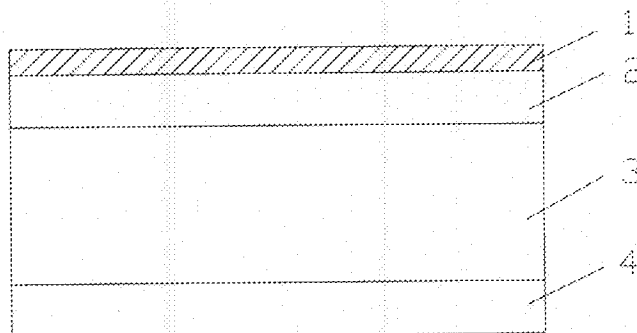
**Figure 3**

The unit cell # 3

1 -  $\text{UO}_2$  (90%),  $\Delta t = 0.173$  cm

3 - Th (met),  $\Delta t = 1.01$  cm

2,4 - Polyethylene ( $\text{CH}_2$ ),  $\Delta t = 0.12$  cm



**Figure 4**

The unit cell # 21

1 -  $\text{UO}_2$  (36%),  $\Delta t = 0.173$  cm

3 - Th (met),  $\Delta t = 1.01$  cm

2,4 - Polyethylene( $\text{CH}_2$ ),  $\Delta t = 0.34$  cm