

Fission of U-238 and Pu-239 production in subcritical sets

P. Karpowicz, University of Warsaw

M. Konieczny, Warsaw University of Technology

Supervisor:

Andrzej Wojciechowski Ph. D.,

Laboratory of Information Technologies (LIT)

Neutrons & Protons

REACTION
SCATTERING
CAPTURE
FISSION
SPALLATION

Uranium & Plutonium

Fission of U-238 and Pu-239 production in subcritical sets

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Problem to solve

The main goal of project is a computer simulation of Quinta experiment, to find out why previous simulations didn't suit experimental results.

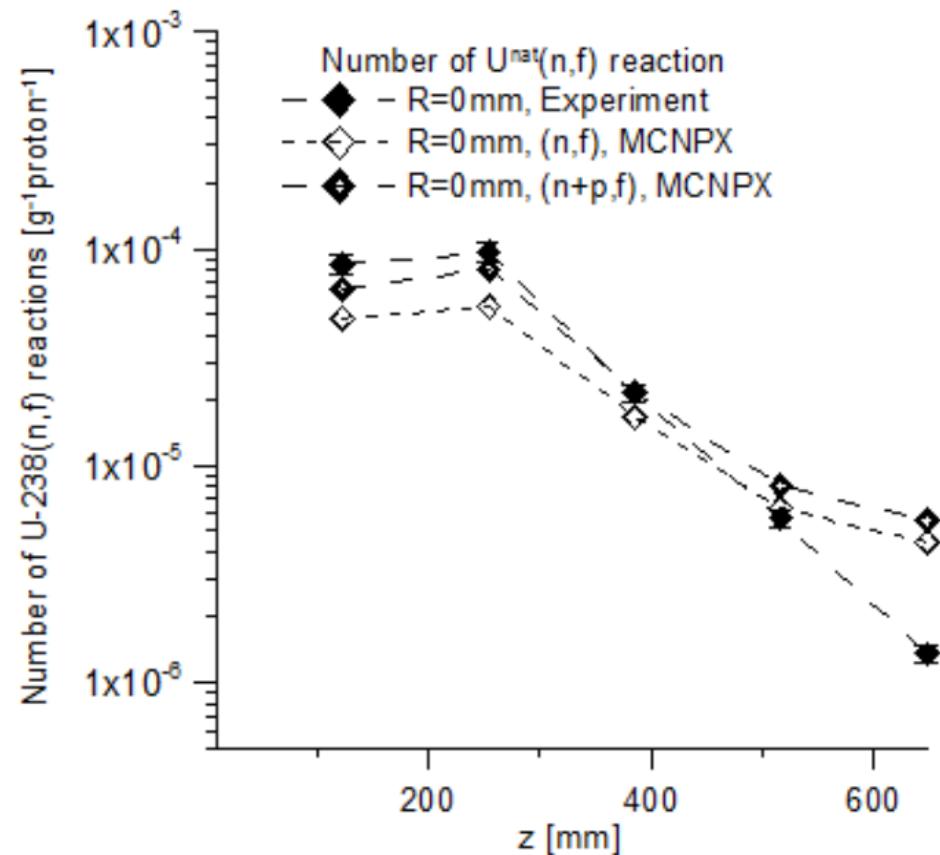


Fig. 1. Comparison of experiment and simulations results.

Quinta experiment

- Experimental data comes from experiment run by prof. Voronko and his group of scientist from Ukraine. Experiment took place in Dzhelepov Laboratory of Nuclear Problems in November 2014 using a PHASOTRON.
- Research connected with particle beam profile was run by Lukas Zavorka from Czech Republic.
- Data from experiment were analyzed in Laboratory of Information Technologies.
- Exercise is based on the results of experimental collaboration „Energy and Transmutation of Radioactive Wastes”.
- Project supervisor: Siergiej Tiutiunnikov.
- Members of a group: Russia (JINR Dubna, CPTP Atomenergomash, Moscow, Russia, Obninsk), Belarus, Poland, Czech Republic, Germany, France, Greece, Mongolia, Ukraine, Australia.

Experiment setup

Layout of upgraded target assembly "Quinta" at the irradiation position

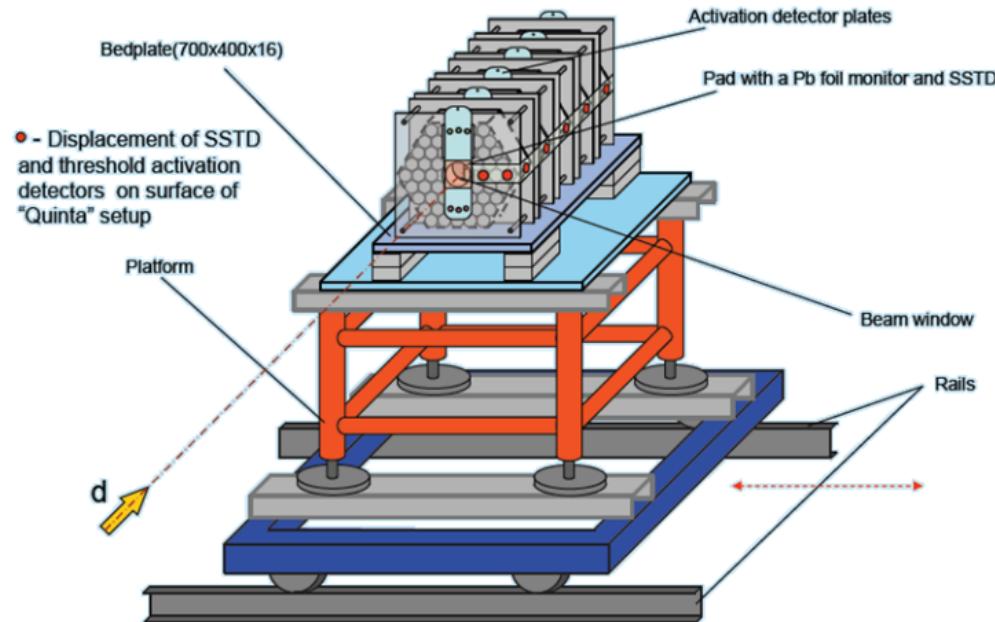


Fig. 2. Quinta experiment setup.

REACTION

**SCATTERING
CAPTURE
FISSION
SPALLATION**

ns
ns

Ura
Plu

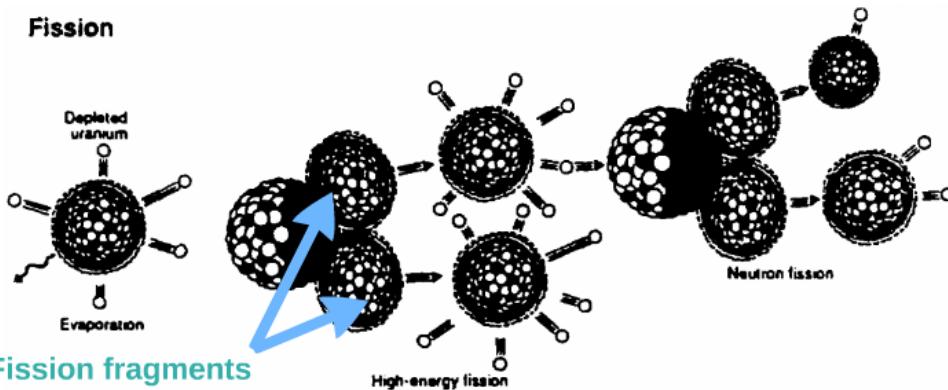
Fig. 1. Comparison of experiment and simulations results.
 1×10^{-6}
200 z [mm] 400

There is a
We calculated
for 5 different ang
.3.32°
.2.47°
.0°
.074°
.1.74°

Fission

Fission is a reaction (decay) of splitting nuclei to lighter parts, with releasing huge amount of energy via neutrons and gamma rays. Reaction can be extorted by neutron flux.

Fission



Fission fragments

High-energy protons bombarding uranium target, high-energy fission competes with evaporation during de-excitation. More neutrons are emitted from high-energy fission than evaporation. Emitted neutrons can go on to induce more fission events.

Fig. 3. Fission scheme.

Fission and spallation happen in the same nucleus!

Spallation

It's obtained by flux of high energy protons hitting a target (lead, mercury). In effect, nucleus emits several nucleons. Spallation is used to produce high beams of neutrons.

Hadronic cascade

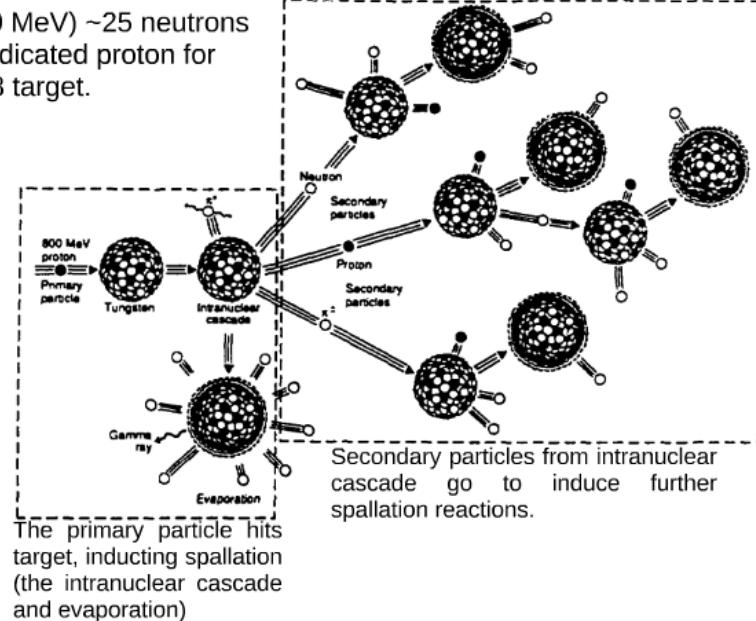


Fig. 4. Spallation scheme.

The cross section for U-238(n,f) reaction sharply increase for energies greater than 1 MeV and peaks for energy equal about 50 MeV. It means that to fission U-238 we must produce neutron with energy greater than 10 MeV.
 (Average energy of fission neutrons is equal to \sim 2 MeV).

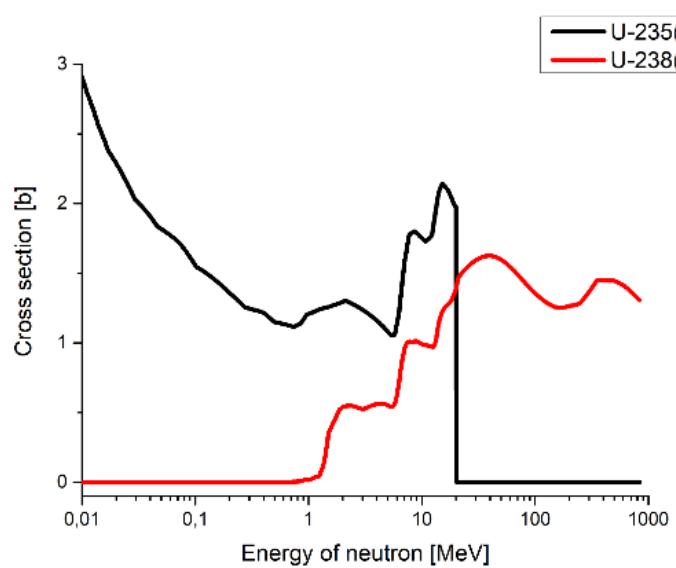


Fig. 5. Cross sections for U-235(n,f) and U-238(n,f).

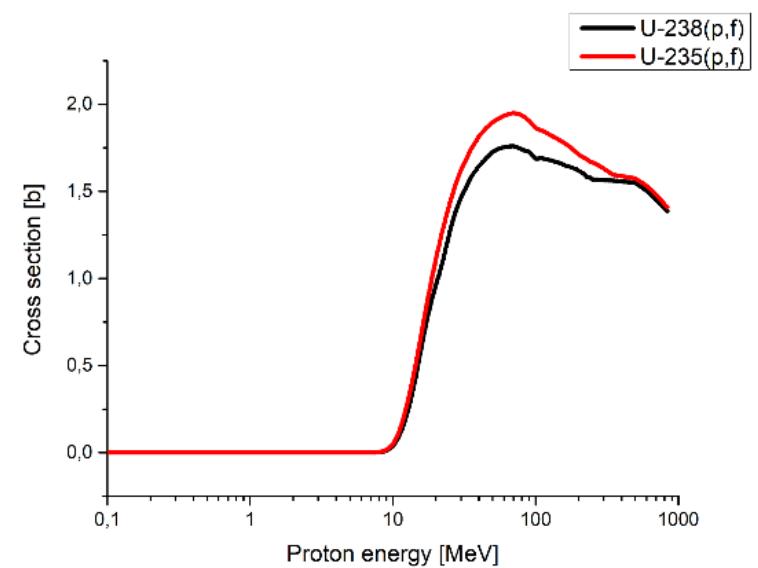


Fig. 6. Cross sections for U-235(p,f) and U-238(p,f).

How to calculate that?

First estimation method

$$Y_{U(n,f)Z} = a_{U235} Y_{U235(n,f)Z} (E_n = 25.3 \text{ meV}) + a_{U238} Y_{U238(n,f)Z} (E_n = 14 \text{ MeV})$$

$$Y_{U(n,f)Z} = (Y_{U238(n,f)Z} (E_n = 0.5 \text{ MeV}) + Y_{U238(n,f)Z} (E_n = 14 \text{ MeV})) / 2$$

Looks fine, but we receive too low precision.

Second estimation method

$$n_{U(x,f)Z}^{\exp} = \int_0^{\infty} (\phi^n(E) \sigma_{U(n,f)Z}(E) + \phi^p(E) \sigma_{U(p,f)Z}(E)) \rho \frac{A}{m} dE$$

To find total fissions number we can convert previous equation into:

$$n_{U(x,f)Z}^{\exp} = \int_0^{\infty} (\phi^n(E) \sigma_{U(n,f)}(E) \frac{\sigma_{U(n,f)Z}(E)}{\sigma_{U(n,f)}(E)} + \phi^p(E) \sigma_{U(p,f)}(E) \frac{\sigma_{U(p,f)Z}(E)}{\sigma_{U(p,f)}(E)}) \rho \frac{A}{m} dE$$

$$n_{U(x,f)Z}^{\exp} = \int_0^{\infty} (\phi^n(E) \sigma_{U(n,f)}(E) Y_{U(n,f)Z} + \phi^p(E) \sigma_{U(p,f)}(E) Y_{U(p,f)Z}) B dE$$

If $Y_{U(p,f)Z}$ and $Y_{U(n,f)Z}$ are constant function of energy one can easily obtain:

$$n_{U(x,f)Z}^{\exp} = Y_{U(n,f)Z} n_{U(n,f)} + Y_{U(p,f)Z} n_{U(p,f)}$$

Measured fission fragments Z were:

- Zr-90
- I-131
- I-133
- Ce-143

How to calculate that?

We can write system of previously equation for measured fission fragments in following matrix form:

$$\begin{bmatrix} n_{Zr97}^{\exp} \\ n_{I131}^{\exp} \\ n_{I133}^{\exp} \\ n_{Ce143}^{\exp} \end{bmatrix} = \begin{bmatrix} Y_{Zr97,U(n,f)} & Y_{Zr97,U(p,f)} \\ Y_{I131,U(n,f)} & Y_{I131,U(p,f)} \\ Y_{I133,U(n,f)} & Y_{I133,U(p,f)} \\ Y_{Ce143,U(n,f)} & Y_{Ce143,U(p,f)} \end{bmatrix} \begin{bmatrix} n_{U(n,f)} \\ n_{U(p,f)} \end{bmatrix}$$
$$\begin{cases} n_{U(n,f)} \geq 0 \\ n_{U(p,f)} \geq 0 \end{cases}$$

The solve of equation system can be transformed to the standard form:

$$\bar{n} = (\bar{Y}^T \bar{Y})^{-1} \bar{Y}^T \bar{n}^{\exp}$$

If we obtain non-physical result it means that experimental error is greater than calculated value. It is when number of proton fissions is significantly less than number of neutron fissions. In that case, we can assume number of proton fissions equal to 0, and we obtain simple explicit form for neutrons fission:

$$n_{U(n,f)} = \frac{\sum_z^4 Y_z n_z^{\exp}}{\sum_z^4 Y_z^2}$$

How to quick calculate that?

Answer:

Computer calculations using
Monte-Carlo method.

Monte Carlo N-Particle eXtended (MCNPX) is a software package for simulating nuclear processes, developed by Los Alamos National Laboratory.

Simple calculations took about 5 days.

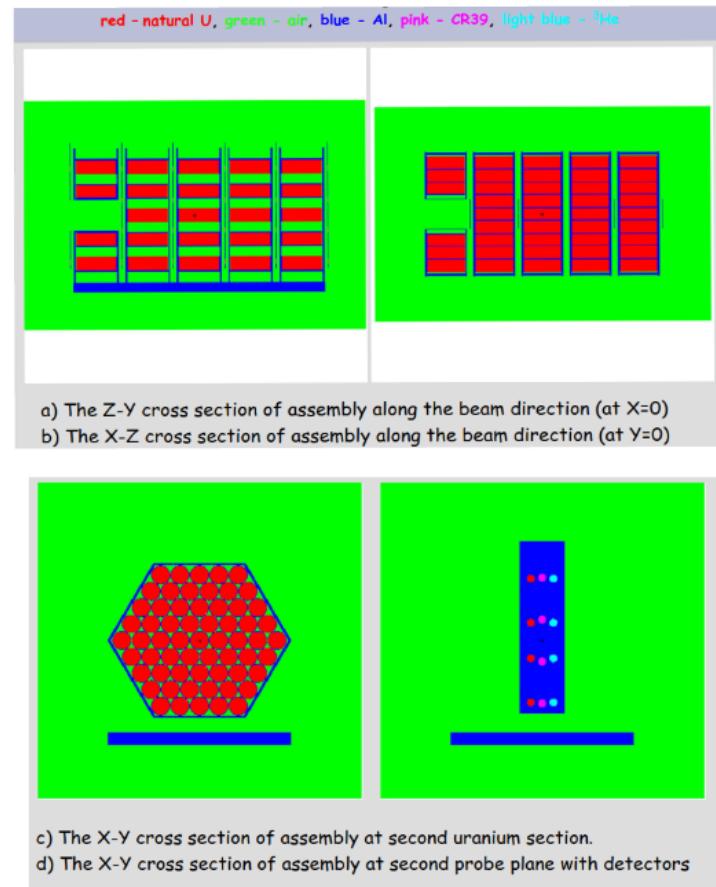
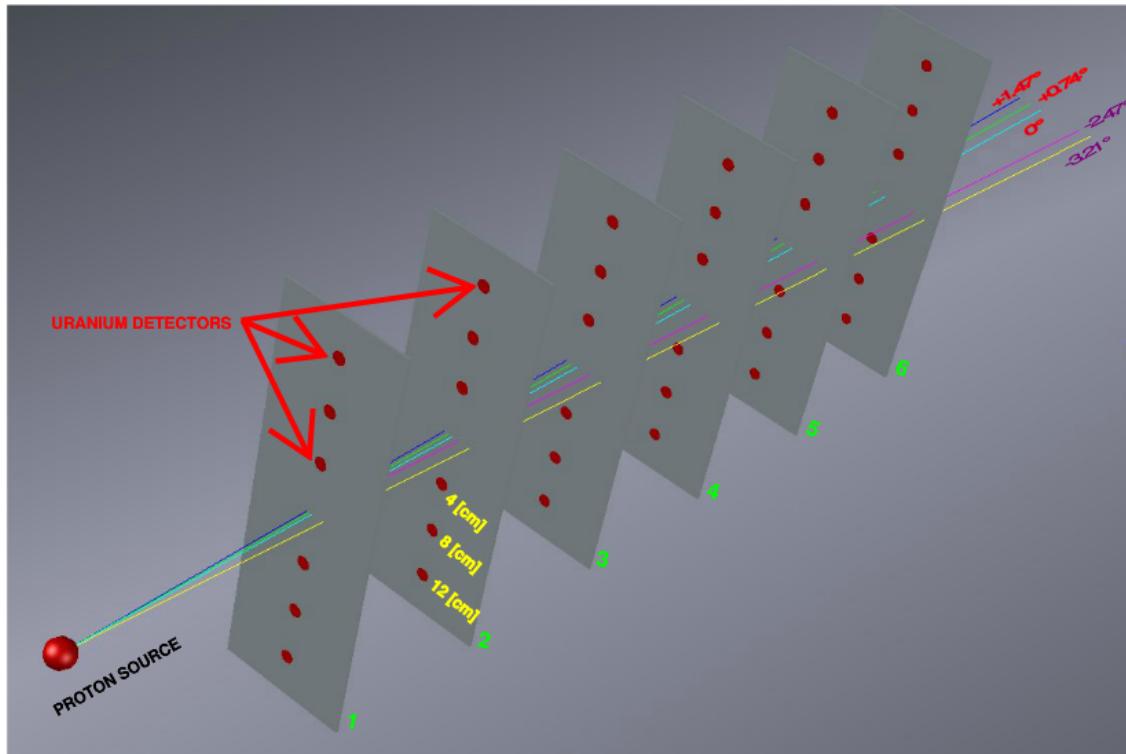


Fig. 7. Geometry of simulation setup.

How to solve our problem

We recognize that beam of protons can be deflected in x axis.



There is also deflection in y-axis, but it is constant and equal 1.84° .

We calculated 5 options
for 5 different angles:

- -3.21°
- -2.47°
- 0°
- 0.74°
- 1.74°

We chose two best cases:

- -3.21°
- -2.47°

And conduct further
analysis for them.

Results

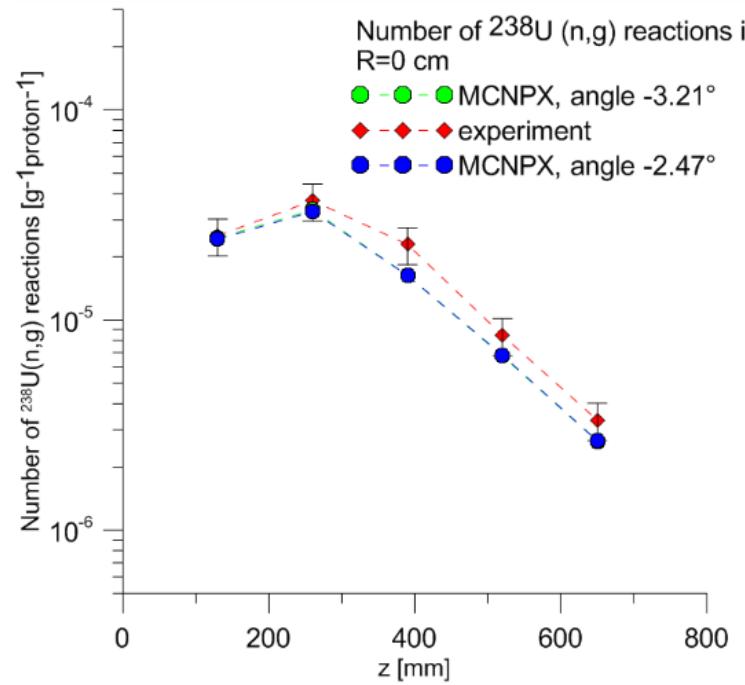
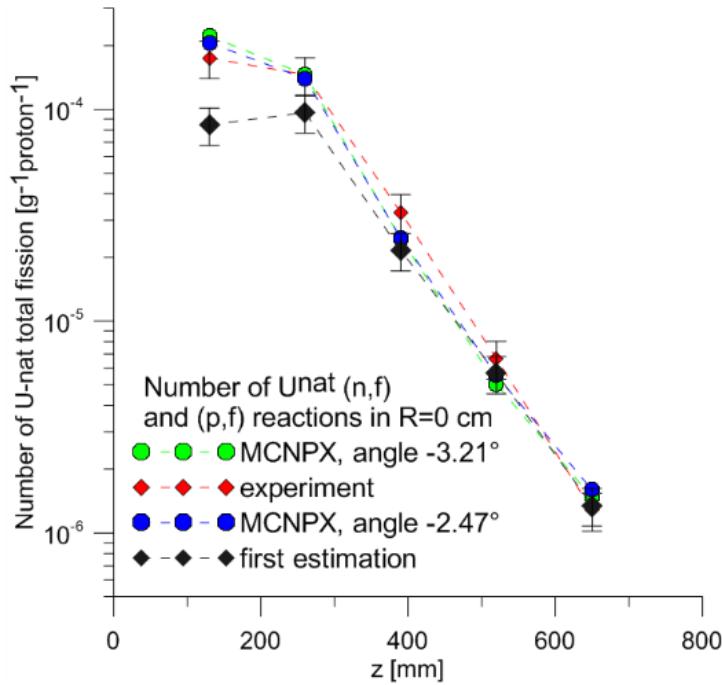


Fig. 8. and Fig. 9.

Results

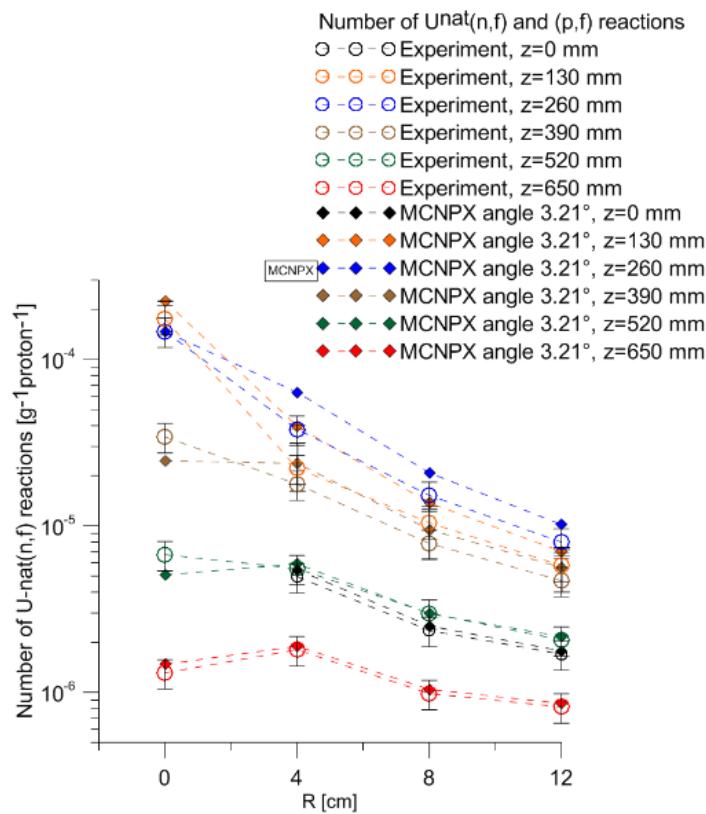


Fig. 10.

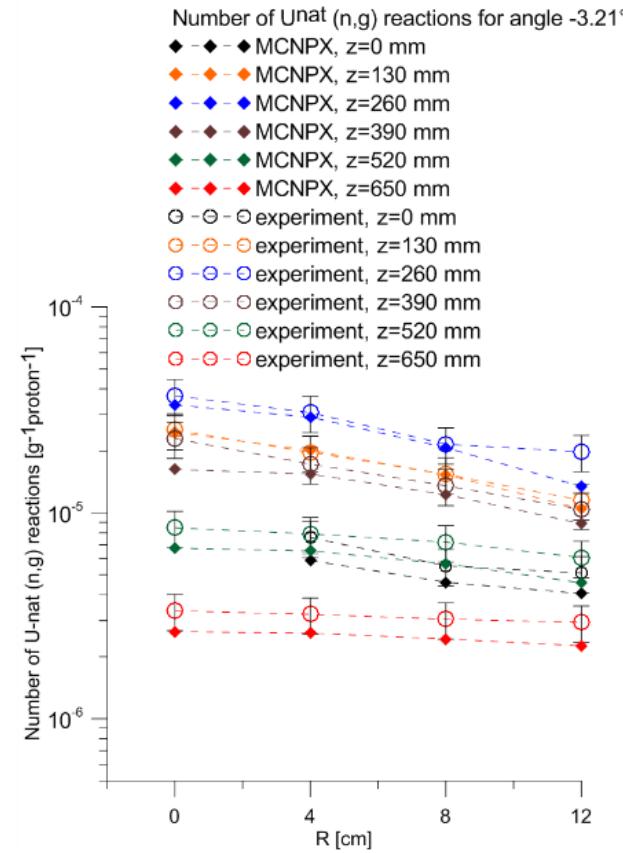


Fig. 11.

Results

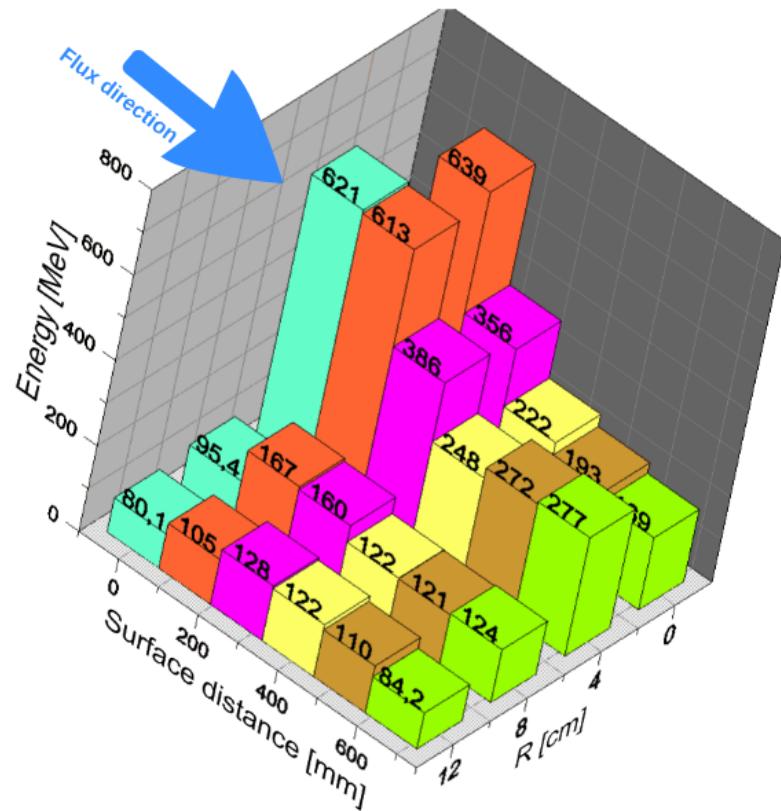


Fig. 12. Average proton energy in detectors for angle = -3.21° .

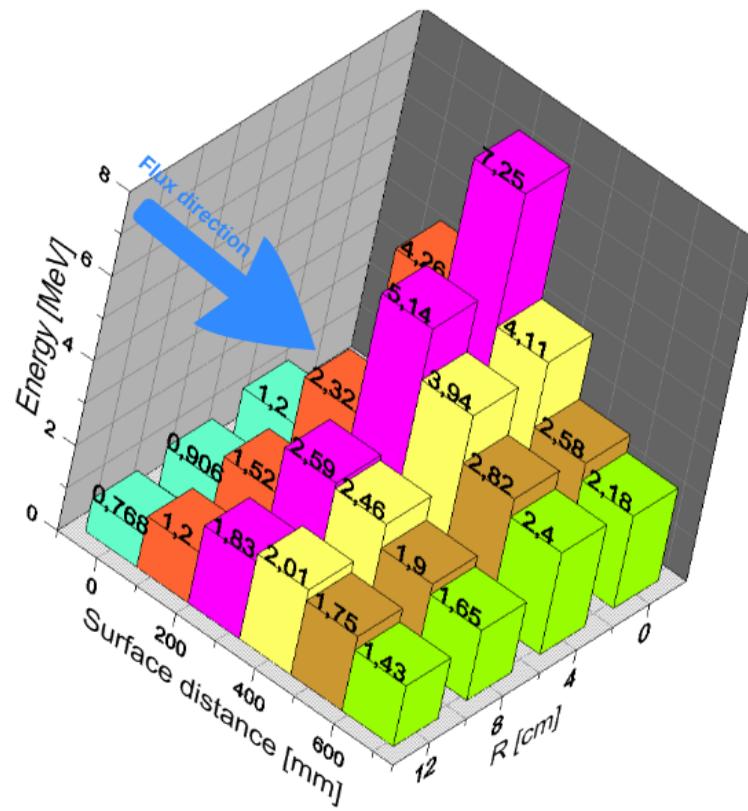
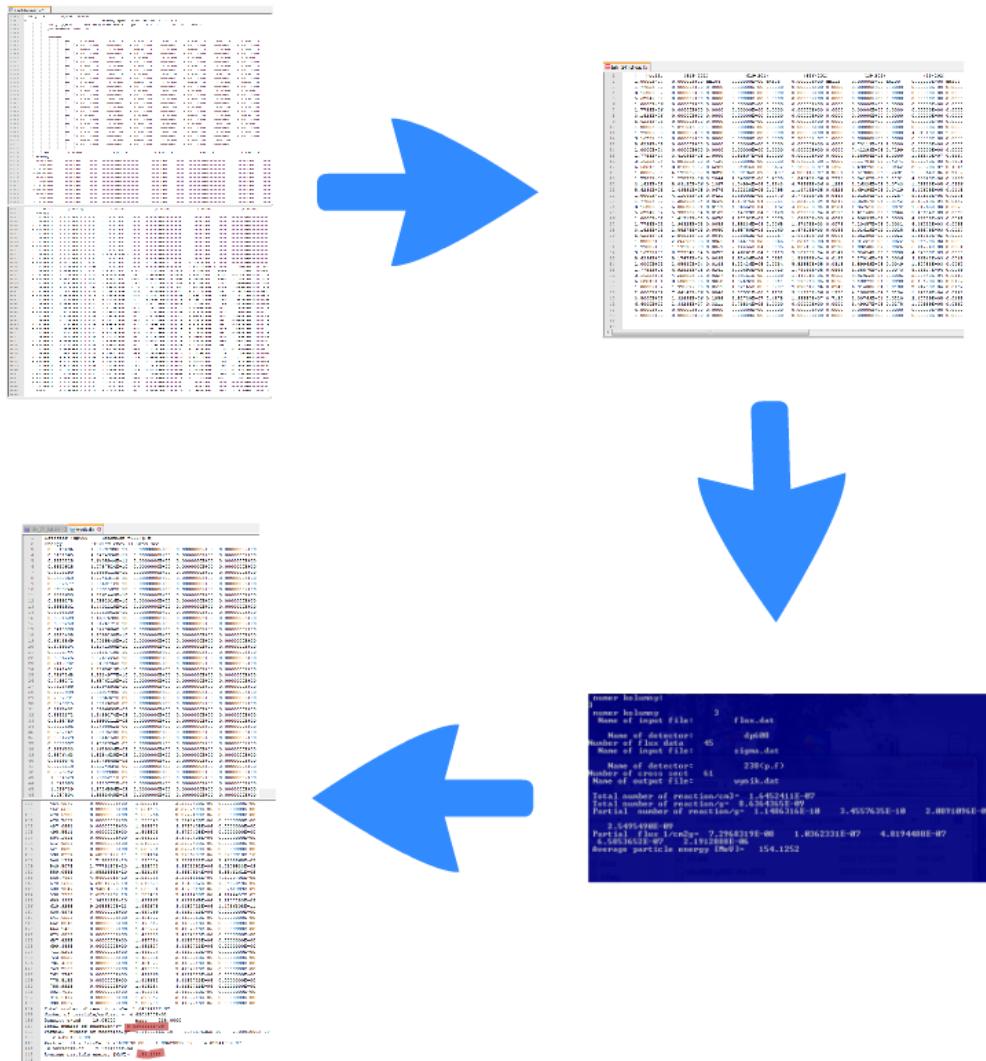


Fig. 13. Average neutron energy in detectors for angle = -3.21° .

In conclusion...

- We succeeded in finding out a possible cause of our problem - deflected beam in x-axis.
- We obtained a good agreement of experimental data and calculated results in all detectors, especially on the assembly axis.
- We estimated angle of deflection to be in range between -3.21° to -2.47° .
- Computer modeling is much easier process than conducting an actual experiment.
- It is also a great tool to predict results and even upgrade experimental data in terms of quality.

What analysis look like - "the kitchen"



tally_24_full.dat						
	cell:	(618<201)	(619<201)	(616<201)	(18<202)	(13<202)
1		1.0000E-07	0.00000E+00	dn104	0.00000E+00	dn108
2		1.7783E-07	0.00000E+00	0.0000	0.00000E+00	0.0000
3		3.1623E-07	0.00000E+00	0.0000	0.00000E+00	0.0000
4		5.6234E-07	0.00000E+00	0.0000	0.00000E+00	0.0000
5		1.0000E-06	0.00000E+00	0.0000	0.00000E+00	0.0000
6		1.7783E-06	0.00000E+00	0.0000	0.00000E+00	0.0000
7		3.1623E-06	0.00000E+00	0.0000	0.00000E+00	0.0000
8		5.6234E-06	0.00000E+00	0.0000	0.00000E+00	0.0000
9		1.0000E-05	4.87691E-08	1.0000	0.00000E+00	0.0000
10		1.7783E-05	0.00000E+00	0.0000	0.00000E+00	0.0000
11		3.1623E-05	0.00000E+00	0.0000	2.38358E-07	1.0000
12		5.6234E-05	0.00000E+00	0.0000	0.00000E+00	0.0000
13		1.0000E-04	0.00000E+00	0.0000	0.00000E+00	0.0000
14		1.7783E-04	3.41096E-08	1.0000	2.53507E-08	1.0000
15		3.1623E-04	6.88155E-08	0.7136	0.00000E+00	0.0000
16		5.6234E-04	3.81885E-07	0.5287	9.34046E-08	0.5672
17		1.0000E-03	6.17136E-07	0.3020	6.89194E-07	0.3487
18		1.7783E-03	1.22829E-06	0.2044	1.54082E-06	0.2305
19		3.1623E-03	5.03120E-06	0.1387	4.04994E-06	0.1343
20		5.6234E-03	1.43591E-05	0.0674	1.22328E-05	0.0795
21		1.0000E-02	4.11069E-05	0.0421	3.69003E-05	0.0470
22		1.7783E-02	1.38390E-04	0.0229	1.17076E-04	0.0251
23		3.1623E-02	5.00523E-04	0.0117	4.36552E-04	0.0132
24		5.6234E-02	5.93318E-04	0.0109	5.14723E-04	0.0120
25		1.0000E-01	1.41215E-03	0.0070	1.17152E-03	0.0079
26		1.7783E-01	1.94329E-03	0.0059	1.55336E-03	0.0068
27		3.1623E-01	2.55279E-03	0.0050	1.95750E-03	0.0060
28		5.6234E-01	2.86914E-03	0.0046	2.08853E-03	0.0057
29		1.0000E+00	2.25592E-03	0.0051	1.56614E-03	0.0065
30		1.7783E+00	1.19115E-03	0.0067	7.14455E-04	0.0095
31		3.1623E+00	8.29354E-04	0.0079	4.46261E-04	0.0119
32		5.6234E+00	5.17473E-04	0.0095	2.51436E-04	0.0152
33		1.0000E+01	2.05440E-04	0.0143	9.22426E-05	0.0234
34		1.7783E+01	6.92929E-05	0.0261	3.00693E-05	0.0413
35		3.1623E+01	4.25800E-05	0.0327	1.99151E-05	0.0500
36		5.6234E+01	3.60306E-05	0.0368	1.92692E-05	0.0541
37		1.0000E+02	1.97567E-05	0.0511	1.02165E-05	0.0787
38		2.0000E+02	7.64149E-06	0.0846	5.07031E-06	0.1102
39		3.5000E+02	1.32496E-06	0.1856	2.51730E-07	0.4578
40		6.6000E+02	2.33238E-07	0.3211	2.73834E-08	1.0000
41		6.8000E+02	0.00000E+00	0.0000	0.00000E+00	0.0000
42		1.0000E+03	0.00000E+00	0.0000	0.00000E+00	0.0000
43		1.0000E+03	0.00000E+00	0.0000	0.00000E+00	0.0000
44						
45						

▶

```
numer kolumny: 3
numer kolumny      3
Name of input file: flux.dat
Name of detector: dp608
Number of flux data 45
Name of input file: sigma.dat
Name of detector: 238(p,f)
Number of cross sect 61
Name of output file: wynik.dat
Total number of reaction/cm3= 1.6452411E-07
Total number of reaction/g= 8.6364365E-09
Partial number of reaction/g= 1.1486316E-10    3.4557635E-10    2.0891096E-09
2.5495490E-09
Partial flux 1/cm2g= 7.2968319E-08    1.0362331E-07    4.8194488E-07
6.5853652E-07    2.1912888E-06
Average particle energy [MeV]= 154.1252
Kosz          n5.dat          2017-07-17 15:10    Plik DAT
bilety        okw660-pINC-drc-3372        2017-07-17 13:44    Plik
```

tally_24_full.dat wynik.dat

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2	Energy	Flux[cm-2MeV-1]	Cros.sec		
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4	0.5131065	4.5474336E-11	0.0000000E+00	0.0000000E+00	0.0000000E+00
5	0.5220215	7.6405944E-11	0.0000000E+00	0.0000000E+00	0.0000000E+00
6	0.5310915	1.0787524E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
7	0.5403190	1.3989113E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
8	0.5497068	1.7246311E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
9	0.5592577	2.0560112E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
10	0.5689746	2.3931507E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
11	0.5788603	2.7361449E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
12	0.5889178	3.0851016E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
13	0.5991501	3.4401215E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
14	0.6095600	3.8013062E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
15	0.6201509	4.1687698E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
16	0.6309258	4.5426171E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
17	0.6418880	4.9229604E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
18	0.6530405	5.3099108E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
19	0.6643869	5.7035848E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
20	0.6759304	6.1041000E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
21	0.6876744	6.5115718E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
22	0.6996225	6.9261225E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
23	0.7117782	7.3478784E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
24	0.7241451	7.7769613E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
25	0.7367268	8.2134977E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
26	0.7495272	8.6576218E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
27	0.7625499	9.1094593E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
28	0.7757989	9.5691499E-10	0.0000000E+00	0.0000000E+00	0.0000000E+00
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30	0.8029915	1.0512626E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
31	0.8169432	1.0996695E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
32	0.8311372	1.1489174E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
33	0.8455780	1.1990211E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
34	0.8602695	1.2499952E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
35	0.8752164	1.3018548E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
36	0.8904229	1.3546158E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
37	0.9058937	1.4082934E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
38	0.9216333	1.4629036E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
39	0.9376463	1.5184625E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
40	0.9539376	1.5749868E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
41	0.9705119	1.6324934E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
42	0.9873742	1.6909988E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
43	1.004529	1.7505211E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
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405	512.9207	0.0000000E+00	1.542273	3.3727408E-06	0.0000000E+00
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409	549.5078	2.7773137E-10	1.525772	3.3801291E-06	4.0109533E-09
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411	568.7687	4.9600241E-10	1.517085	3.3931556E-06	7.3720705E-09
412	578.6509	5.2064797E-10	1.512628	3.4010052E-06	7.8497049E-09
413	588.7047	3.9405498E-10	1.508094	3.4070313E-06	6.0261809E-09
414	598.9333	2.6526176E-10	1.503481	3.4111458E-06	4.1144457E-09
415	609.3395	1.3423132E-10	1.498162	3.4132565E-06	2.1107183E-09
416	619.9266	9.2453540E-13	1.492678	3.4132713E-06	1.4736308E-11
417	630.6976	0.0000000E+00	1.487099	3.4132713E-06	0.0000000E+00
418	641.6557	0.0000000E+00	1.481422	3.4132713E-06	0.0000000E+00
419	652.8042	0.0000000E+00	1.475647	3.4132713E-06	0.0000000E+00
420	664.1465	0.0000000E+00	1.469772	3.4132713E-06	0.0000000E+00
421	675.6858	0.0000000E+00	1.463795	3.4132713E-06	0.0000000E+00
422	687.4255	0.0000000E+00	1.457714	3.4132713E-06	0.0000000E+00
423	699.3693	0.0000000E+00	1.451527	3.4132713E-06	0.0000000E+00
424	711.5206	0.0000000E+00	1.445774	3.4132713E-06	0.0000000E+00
425	723.8830	0.0000000E+00	1.439951	3.4132713E-06	0.0000000E+00
426	736.4602	0.0000000E+00	1.434027	3.4132713E-06	0.0000000E+00
427	749.2560	0.0000000E+00	1.428000	3.4132713E-06	0.0000000E+00
428	762.2740	0.0000000E+00	1.421869	3.4132713E-06	0.0000000E+00
429	775.5182	0.0000000E+00	1.415631	3.4132713E-06	0.0000000E+00
430	788.9926	0.0000000E+00	1.409284	3.4132713E-06	0.0000000E+00
431	802.7010	0.0000000E+00	1.402841	3.4132713E-06	0.0000000E+00
432	816.6477	0.0000000E+00	1.396342	3.4132713E-06	0.0000000E+00
433	830.8367	0.0000000E+00	1.389730	3.4132713E-06	0.0000000E+00
434	Total number of reaction/cm3= 1.6452411E-07				
435	Number of particle/cm*barn = 4.8201300E-02				
436	Density g/cm3= 19.05000 masa= 238.0000				
437	Total number of reaction/g= 8.6364365E-09				
438	Partial number of reaction/g= 1.1486316E-10 3.4557635E-10 2.0891096E-09 2.5495490E-09				
439	Partial flux 1/cm2= 7.2968319E-08 1.0362331E-07 4.8194488E-07 6.5853652E-07 2.1912888E-06				
440	Average particle energy [MeV]= 154.1252				
441					
442					
443					

THANK YOU!

And we hope we resolved all your doubts

Sources

- Spallation Physics - An Overview, Gary J. Russel
- Neutron Generation, John M. Carpenter
- Users manual for MCNPX 2.7.0