



## Maximum Likelihood Estimation of a Neutron Spectrum and Associated Uncertainties

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### Abstract:

*This article discusses several methods for computing neutron (resp. gamma) spectrum from experimental data. In addition to basic description, we also outline the possibilities of propagation of uncertainty. In detail we describe the Maximum Likelihood Estimation, which we have applied to computing neutron and gamma spectra from experimental data. Moreover, we have found a procedure to determine the uncertainty of the resulting spectrum.*

### Keywords:

*Unfolding, maximum likelihood estimation, uncertainty propagation*

### 1. Notation

- $\mathbf{x}$  - vector (Vectors are printed in bold.)
- $E(X)$  - expected value of  $X$
- $\mathbf{C}_g$  - covariance matrix of random vector  $\mathbf{g}$
- $Po(I)$  - Poisson distribution with parameter  $I$ .

### 2. Problem Formulation

When evaluating experimental data, we often meet so called *deconvolution* or *unfolding* problem that can be generally formulated as follows: Let  $g(x)$  and  $A(x, y)$  be (continuous) functions. A (continuous) function  $f(y)$  is to be found such that

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$$g(x) = \int_{(I)} A(x, y) f(y) dy \quad (1)$$

The above equation models the process of measurement using various devices or e.g. the output of a graphical device. It is a Fredholm integral equation of the first kind where

- $A(x, y)$  is the *convolution kernel*, a characteristic of the measuring device, often called the *response function*,
- $g(x)$  is the experimental data, and
- $f(y)$  is the result to be found,
- $I$  is interval of energies.

When applied to spectrometry, the following issues arise:

- In general, there is no analytic solution to the equation (1).
- The response function  $A(x, y)$  of the measuring device has to be determined. It can be done by combination of stochastic (or deterministic) computation with an experiment. The uncertainties associated with function  $A$  are usually very hard to find.

Equation (1) has to be solved in discrete form

$$\mathbf{g} = \mathbf{A}\mathbf{f}, \quad (2)$$

where  $\mathbf{g} = (g_1, \mathbf{K}, g_m)^T$ ,  $\mathbf{A}$  is a  $m \times n$  matrix, and  $\mathbf{f} = (f_1, \mathbf{K}, f_n)^T$ . ( $T$  means transposition.) In further text, we examine the case  $m = n$  since it is relevant for stilbene and NE-213 detectors etc. In this case,  $m \approx 10^3$ .

The interpretation of  $\mathbf{f}$ ,  $\mathbf{g}$ , and  $\mathbf{A}$  is the following:

- $\mathbf{g}$  is the measured proton (resp. electron) spectrum, i.e. experimental data. (Neutrons are detected by means of protons and photons by means of electrons.)
- $\mathbf{A}$  is the detector response function. It is determined by the Monte Carlo method and measurement of monoenergetic sources of neutrons and photons.
- $\mathbf{f}$  is the resulting neutron (resp. gamma) spectrum to be found. (The unit of  $\mathbf{f}$  is  $\text{m}^{-2} \text{s}^{-1} \text{MeV}^{-1}$ .)

The linear system (2) cannot be solved by usual procedures since the matrix  $\mathbf{A}$  is usually ill-conditioned. The determinant of our matrix response function for detector  $20 \times 20$  mm is  $|\mathbf{A}| \approx 3 \cdot 10^{-133}$ . The resulting neutron (resp. gamma) spectrum has to satisfy a few conditions originating from its physical properties; above all, non-negativity is required:  $f_i \geq 0, 1 \leq i \leq n$ .

### Remark

The evaluation of neutron and gamma spectra is very similar. In the following text, all the information about neutron (resp. proton) spectra also applies to gamma (resp. electron) spectra unless it is explicitly indicated otherwise.

### 3. Overview of Unfolding Methods

#### 3.1. Direct Inverse

The simplest way to get the neutron spectrum  $\mathbf{f}$  is the direct inverse of the response matrix:

$$\mathbf{f} = \mathbf{A}^{-1} \mathbf{g} \quad (3)$$

Because the system is ill-conditioned, such solution is unstable<sup>1</sup>. Although the stability of the solution can be improved by e.g. *singular value decomposition* method, its non-negativity cannot be simply guaranteed.

#### 3.2. Differentiation Method

Let us presume about the response function  $A(x, y)$  that it does not depend on the energy of the scattered proton  $x$ . Then, equation (1) can be differentiated and the neutron spectrum expressed as

$$f(y) = - \frac{y}{e_k(y)} \left. \frac{dg(x)}{dx} \right|_{x=y}, \quad (4)$$

where  $e_k(y)$  is the detection efficiency with threshold  $k$ .

The main advantage of this method is, besides its simplicity, the possibility to change the energetic scale easily. The main disadvantage is its very low stability, i.e. sensitivity to small changes in input data. It is advisable to fit a smooth function to the input data before application of this method.

The importance of this method has been decreased with computer development.

#### 3.3. Least Squares

##### Linear Model

If the least squares method is used for unfolding, we have to distinguish two phases: adjustment and the solution itself.

The adjustment of the deconvolution procedure means minimizing the expression

$$c^2 = (\mathbf{g} - \mathbf{A}\mathbf{f})^T \mathbf{C}_g^{-1} (\mathbf{g} - \mathbf{A}\mathbf{f}), \quad (5)$$

where  $\mathbf{C}_g$  is the covariance matrix of the measured proton spectrum [1].

Equation (5) can be further extended with another two elements that insert prior information about the neutron spectrum and about the response matrix when it is parametrized by properties of the proton spectrum.

The solution is unique but the formula is rather complex. The non-negativity condition cannot be guaranteed by linear model and the prior information about the neutron spectrum has to be good for the method to be usable at all. (See [1] where the least squares method is discussed thoroughly.)

Examples of unfolding routines using the linear least squares method include STAY'SL [2], LEPRICON [3], MSITER and MINCHI [4].

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<sup>1</sup> with small change of  $\mathbf{g}$ ,  $\mathbf{f}$  changes a lot

### Non-linear Model

If we want to ensure non-negativity of the solution, the non-linear model has to be applied. The expression to be minimized depends on concrete model but generally, it is similar to the right-hand side of equation (5).

This method results in an iteration process that secures the non-negativity condition and is able to employ prior information. Instead of computing components  $f_i$  of the neutron spectrum directly, their logarithms or squares are evaluated. The main disadvantage is the possibility of oscillations (mainly when the number of iterations is high) which means that the result may be significantly influenced by number of iterations.

The non-linear model is used by e.g. SAND-II [5], GRAVEL [6], and LOUHI [7].

### Linear Regularization

The method of linear regularization ([8], [9]) comes out from the natural requirement that the spectrum values in adjacent energetic groups should not oscillate much; they should rather tie together.

Therefore, we extend the minimized  $c^2$  expression with some criterion  $S$  for "smoothness" of the solution:

$$c^2 + aS, \quad (6)$$

where  $a$  is a parameter (real number). If chosen  $a \approx 0$ , we might obtain oscillating solutions that satisfy the  $c^2$  criterion very well. On the other hand, bigger values of  $a$  result in unrealistically smooth neutron spectra.

Another degree of freedom is the expression  $S$ . A common choice is

$$S \equiv \sum_{i=2}^{n-1} (2f_i - f_{i+1} - f_{i-1})^2, \quad (7)$$

which is the discrete form of

$$\int_M [f''(x)]^2 dx.$$

This is known as *Tikhonov regularization*.

### 3.4. Maximum Entropy

The maximum entropy solves the unfolding problem in the following way: we consider the neutron spectrum a  $n$ -dimensional random vector. Let the parameters of the probability distribution function depend on the proton spectrum  $\mathbf{g}$  and the response matrix  $\mathbf{A}$ . Then we take the expected value of this distribution as the resulting neutron spectrum.

### Notice

This approach is especially efficient in *few-channel* spectrometry. The response matrix is strongly rectangular, i.e. the dimension of the neutron spectrum is much higher than the dimension of the proton spectrum:  $\dim(\mathbf{f}) \gg \dim(\mathbf{g})$ . The space of possible solutions to equation (2) is immense and the selection of one particular neutron spectrum is complicated.

It is known from statistics and information theory [10] that a random vector prefers such probability density  $P(\mathbf{x})$  that maximizes the entropy defined as

$$S = -\int_N P(\mathbf{x}) \log(P(\mathbf{x})) dx \quad (8)$$

Now two questions arise:

1. What kind of probability distribution to choose?
2. How to incorporate the information about the proton spectrum and response function (matrix) into the parameters of the distribution?

### Multivariate Normal Distribution

The first distribution that has been used is the multivariate normal distribution. Its density function takes the form

$$P(\mathbf{x}) = C_1 \exp\left(-a c^2/2\right), \quad (9)$$

where

- $C_1$  is a normalizing constant,
- $c^2 = (\mathbf{Ax} - \mathbf{g})^T \mathbf{C}_g^{-1} (\mathbf{Ax} - \mathbf{g})$ ,
- the parameter  $a$  can be obtained from the condition  $E(c^2) = n$  (e.g. by means of Monte Carlo method).

Computation of the expected value (which is a vector) is quite complicated for this distribution and numerical methods have to be used. For example, the MIEKE code [6] uses a Monte Carlo approach with importance sampling. The resulting neutron spectrum is estimated as

$$\mathbf{f} = \frac{1}{N} \sum_{j=1}^N \mathbf{f}^j, \quad (10)$$

where  $N$  is the number of generated samples and  $\mathbf{f}^j$  is the  $j$ -th sample.

### Multivariate Exponential Distribution

When the normal distribution is replaced with exponential, the computations become much simpler [10]. The probability density can be expressed as

$$P(\mathbf{x}) = C_2 \exp\left(-\mathbf{b}^T \mathbf{Ax}\right), \quad (11)$$

where

- vector  $\mathbf{b}$  is obtained as the solution to a simple non-linear system
- $C_2 = \prod_{k=1}^n (\mathbf{A}^T \mathbf{b})_k$

The expected value  $\mathbf{f}$  can be computed easily:

$$f_i = 1/(\mathbf{A}^T \mathbf{b})_i, \quad 1 \leq i \leq n \quad (12)$$

Further, Weise [11] has proved that for  $n \rightarrow \infty$  the expected values are identical for both distributions (9) and (11). The UNFANA code works in this way [11].

### 3.5. Maximum Likelihood Estimation

The maximum likelihood estimation is a standard statistical tool for point estimations. For the maximizing of the likelihood function, we use a general iterative algorithm called *Expectation Maximization* (EM in further text), originally developed for image reconstruction in astronomy, medicine etc.

#### Model Description

As outlined in the introduction, theoretically both proton and neutron spectrum are continuous functions. On the other hand, the measuring device allows measuring the values of the proton spectrum only in finitely many points; thus, we divide the real axis into finitely many (usually equidistant) energetic intervals (groups).

Experiments show that if the energetic intervals are narrow enough then the number of particles with energy falling into an interval has the Poisson distribution. Therefore, it is natural to model the proton (and neutron) spectrum with a random vector with Poisson distributed components. For the purpose of simplification, we can further assume that the components are mutually independent.

#### Derivation of the EM Algorithm

Let us presume that the neutron spectrum is a random vector  $\hat{\mathbf{f}} = (\hat{f}_i, \mathbf{K}, \hat{f}_n)^T$  which satisfies

1.  $\hat{f}_i \sim Po(f_i)$ , i.e. the  $i$ -th component of  $\hat{\mathbf{f}}$  is a Poisson distributed random variable with (unknown) parameter  $f_i$ ; thus, the probability mass function

$$\text{(PMF) of component } \hat{f}_i \text{ is } e^{-f_i} \frac{f_i^{x_i}}{x_i!}. \quad (x_i \text{ is the independent variable.})$$

2. The components of  $\hat{\mathbf{f}}$  are mutually independent.

Corollary: The joint PMF of vector  $\hat{\mathbf{f}}$  can be expressed as

$$F(x_1, \mathbf{K}, x_n) = \prod_{i=1}^n e^{-f_i} \frac{f_i^{x_i}}{x_i!}. \quad (13)$$

If we consider the proton spectrum  $\mathbf{g}$  a random vector  $\hat{\mathbf{g}} = (\hat{g}_i, \mathbf{K}, \hat{g}_n)^T$  and  $a_{ij}$  are components of the response matrix, we can write

$$\hat{g}_i = \sum_{j=1}^n a_{ij} \hat{f}_j, \quad 1 \leq i \leq n. \quad (14)$$

Thanks to properties of Poisson distribution we obtain

1.  $\hat{g}_i$  is a Poisson distributed random variable with parameter  $\bar{g}_i = \sum_{j=1}^n a_{ij} f_j$
2. The components of  $\hat{\mathbf{g}}$  are mutually independent. (Matrix multiplication is a linear transformation.)

The realization of random vector  $\hat{\mathbf{g}}$  is the measured proton spectrum  $\mathbf{g}$ . The *likelihood function* of parameters  $\mathbf{f} = (f_1, \mathbf{K}, f_n)^T$  for  $\mathbf{g}$  is therefore

$$L(\mathbf{f}) = \prod_{i=1}^n e^{-\bar{g}_i} \frac{\bar{g}_i^{g_i}}{g_i!}. \quad (15)$$

The resulting neutron spectrum  $\mathbf{f}$  is the one that maximizes (15). Obviously, instead of maximizing (15) directly, its logarithm can be maximized:

$$l(\mathbf{f}) = \ln(L(\mathbf{f})) = -\sum_{i=1}^n \sum_{j=1}^n a_{ij} f_j + \sum_{i=1}^n g_i \ln \left( \sum_{j=1}^n a_{ij} f_j \right) - \sum_{i=1}^n \ln(g_i!) \quad (16)$$

For further simplification, the response matrix can be normalized:

$$\sum_{i=1}^n a_{ij} = 1, \quad 1 \leq j \leq n. \quad (17)$$

In this case, it can be shown [12] that the sufficient conditions for  $l(\mathbf{f})$  to be maximized by  $\boldsymbol{\mu} = (\mathbf{m}_1, \mathbf{K}, \mathbf{m}_n)^T$  have the form

$$0 = f_i \left. \frac{\partial l(\mathbf{f})}{\partial f_i} \right|_{\boldsymbol{\mu}} = -\mathbf{m}_i + \mathbf{m}_i \sum_{j=1}^n \frac{g_j a_{ji}}{\sum_{k=1}^n \mathbf{m}_k a_{jk}} \quad (18)$$

and

$$\left. \frac{\partial l(\mathbf{f})}{\partial f_i} \right|_{\boldsymbol{\mu}} \leq 0, \quad \text{if } \mathbf{m}_i = 0 \quad (19)$$

for each  $1 \leq i \leq n$ . From equation (18) we can easily get the iteration formula for the EM algorithm:

$$\boxed{f_i^{(k+1)} = f_i^{(k)} \frac{\sum_{j=1}^n g_j a_{ji}}{\sum_{l=1}^n f_l^{(k)} a_{jl}}} \quad (20)$$

The following properties of the EM algorithm can be proved [13]:

1. The EM algorithm converges. Moreover, for each  $k$  we get  $l(\mathbf{f}^{(k)}) < l(\mathbf{f}^{(k+1)})$ .
2. If the initial approximation  $\mathbf{f}^{(0)}$ , the whole response matrix  $\mathbf{A}$ , and the proton spectrum  $\mathbf{g}$  are non-negative, so are all the approximations  $\mathbf{f}^{(k)}$ .
3. For each approximation  $\mathbf{f}^{(k)}$

$$\sum_{i=1}^n f_i^{(k)} = \sum_{j=1}^n g_j, \quad (21)$$

which means that the sum of impulses remains constant over all steps, i.e. the algorithm only re-distributes them among different energetic groups.

#### 4. Propagation of Uncertainties

The uncertainties of the computed neutron spectrum should, above all, include:

- Uncertainties originating from the measured proton spectrum. Among others, the following contributions can be identified:
  - Uncertainties resulting from the stochastic nature of the measurement.
  - Uncertainties resulting from operation of the measuring device.
  - In case of sources with variable emission, the uncertainties resulting from output monitoring have to be included.
  - Uncertainties caused by energetic calibration.
- Possible uncertainties inserted by unfolding. (It does not have to be deterministic.)
- Uncertainties of the response matrix originating from the data and computational model used.
- Uncertainties of the prior information about neutron spectrum (in few-channel spectrometry).

In general, uncertainties can be evaluated in two ways:

1. Standard usage of the error propagation law. This procedure requires an unambiguous, analytically expressed, and roughly linear relation between proton and neutron spectrum. The advantages include low computational complexity and possibility to evaluate the contributions of each source of uncertainty. The main disadvantage consists in limited applicability for iterative unfolding methods. If the relation between proton and neutron spectrum does not satisfy one of the above conditions, it is sometimes possible to simulate it with appropriate function satisfying all of them.
2. Monte Carlo method. In this case, we generate random modifications of input data such that the modifications represent possible variations of the input data in the range of their uncertainties. For each generated sample the corresponding result is computed. The final uncertainties (variance, confidence intervals etc.) are estimated using all of these results. This procedure enables the evaluation of type A uncertainties regardless of the unfolding method used; when the number of generated samples is sufficiently high, the computed uncertainties are very truthful. However, the computing complexity is often high and there is no possibility to evaluate the contributions of each source of uncertainty.

#### Notice

Uncertainties of type B, which cover e.g. the systematic overrating or underrating of the measurement result, can be evaluated by means of very sophisticated measurements in referential emission fields and comparison with computed results.

In the following text, we outline the methods for uncertainty propagation for different unfolding procedures. Methods based on direct inverse will not be discussed as they are unusable for our concerns. Least squares methods are thoroughly inspected in [1]. Therefore, only a brief summary is provided.

#### 4.1. Least Squares

##### Linear Model

The covariance matrix for the neutron spectrum can be computed quite easily. It is possible for it to include uncertainties of the response matrix as well as uncertainties of the prior information  $\mathbf{f}_0$ . The exact formulas are rather complex and can be found e.g. in [1].

##### Non-linear Model and Regularization

The solution is obtained using an iteration process; because of that, the relation between the measured proton spectrum and the computed neutron spectrum is not transparent. The standard formulas for uncertainty propagation cannot be used.

#### 4.2. Maximum Entropy

When using this procedure, the uncertainties of the resulting neutron spectrum consist of two parts: uncertainties originating from input data (i.e. proton spectrum, response matrix, and prior information) and uncertainties caused by the stochastic nature of the unfolding process.

##### Multivariate Normal Distribution

The covariance matrix of the distribution (and thus of the neutron spectrum) can be evaluated by a Monte Carlo approach. If we keep the notation of equation (10), the estimation can be expressed as

$$\mathbf{C}_f = \frac{1}{N-1} \sum_{j=1}^N (\mathbf{f}^j - \mathbf{f})(\mathbf{f}^j - \mathbf{f})^T. \quad (22)$$

The covariance matrix describing the ambiguity of the solution has the form

$$\mathbf{C}_{\text{am}} = \mathbf{C}_f - a^2 \mathbf{C}_f \mathbf{B} \mathbf{C}_f, \quad (23)$$

where  $\mathbf{B} = \mathbf{A}^T \mathbf{C}_g^{-1} \mathbf{A}$ .

##### Multivariate Exponential Distribution

The covariance matrix can be computed much more easily than in the previous case; a (not very complicated) linear system has to be solved. Exact formulas can be found in [12]. On the other hand, there is no simple way to express the ambiguity of the solution.

#### 4.3. Maximum Likelihood Estimation

The uncertainties of the neutron spectrum can be evaluated using the Monte Carlo method. From section 2.5 we know that the neutron spectrum is modelled as a random vector with Poisson distributed, mutually independent components. Therefore, the covariance matrix of the neutron spectrum is diagonal, i.e. it can be replaced with a vector of variances of the components  $\boldsymbol{\sigma}^2 = (s_1^2, \mathbf{K}, s_n^2)$ . To get the estimator  $\mathbf{s}^2 = (s_1^2, \mathbf{K}, s_n^2)$  of  $\boldsymbol{\sigma}^2$ , we repeat the following procedure (for  $j = 1, \mathbf{K}, N$ ):

1. Generate the vector  $\mathbf{g}^j = (g_1^j, \mathbf{K}, g_n^j)$  of pseudorandom numbers from Poisson distribution:  $g_i^j \sim Po(\bar{g}_i)$ .

2. Compute the corresponding neutron spectrum  $\mathbf{f}^j$  (using the MLE-EM algorithm).
3. Store the spectrum  $\mathbf{f}^j$  into memory.

The components of  $\mathbf{s}^2$  can be then computed as

$$s_i^2 = \frac{1}{N-1} \sum_{j=1}^N (f_i^j - f_i)^2, \quad 1 \leq i \leq n. \quad (24)$$

( $f_i$  stands for the  $i$ -th component of the resulting neutron spectrum.)

### Remarks

- Practical usage of this approach shows that the uncertainties can be estimated very well when we generate several tens of vectors  $\mathbf{g}^j$  (i.e.  $N \approx 50$ ). A higher number of samples is not necessary because the computed uncertainties do not change considerably anymore. Today's personal computers complete such a task in several minutes.
- There are many degrees of freedom in the requirement that the generated samples  $\mathbf{g}^j$  "represent possible variations of the input data in the range of their uncertainties". For example, the following constraints can be applied to fulfill this requirement at least partially:
  - For each  $\mathbf{g}^j$  the following must hold:

$$\sum_{i=1}^n g_i^j \approx \sum_{i=1}^n g_i, \quad (25)$$

i.e. the sum of impulses of  $\mathbf{g}^j$  is about the same as in the real measured proton spectrum  $\mathbf{g}$ . Our experience shows that this condition holds implicitly. This is secured by high number of impulses in the energetic groups (thousands and more); the differences up and down in the individual groups balance so that the total sum of impulses is always approximately the same.

- Similarly to the regularization method, it is natural to require that the spectrum values in adjacent energetic groups should not oscillate much; they should rather tie together. This condition also holds implicitly because the variability of number of impulses in a certain energetic group is very small (compared to the average number of impulses generated for this group).

### Uncertainties of the Integral Flux

The *integral flux* is a quantity defined for a given  $I \subseteq \{1, 2, \mathbf{K}, n\}$  as

$$\hat{IF} = \sum_{i \in I} \hat{f}_i. \quad (26)$$

It can be estimated by the expression

$$IF = \sum_{i \in I} f_i. \quad (27)$$

The uncertainties of the integral flux can be evaluated using the stored computed neutron spectra samples  $\mathbf{f}^j$ . The variance can be estimated as

$$s_{IF}^2 = \frac{1}{N-1} \sum_{j=1}^N \left( \sum_{i \in I} f_i^j - \sum_{i \in I} f_i \right)^2. \quad (28)$$

## 5. Conclusion

Based on the EM algorithm, which was adjusted for the purposes of neutron and photon spectrometry, the codes NEUTRONY2 and GAMMA2 have been created using Mathematica 4.1, a system for computer algebra. They take the instrumental separation of neutron and photon impulses according to their energy. The separation is obtained using a two-parameter measuring system described in [14].

The NEUTRONY2 code evaluates data measured by cylindrical stilbene detector sized 10x10 mm, 20x20 mm, and 45x45 mm in the energetic range 0.1-15 MeV. The neutron response matrices for respective detectors were computed by Monte Carlo method; for several neutron energies, they were experimentally verified in PTB Braunschweig [15]. For the 45x45 mm detector it is possible to measure and evaluate the neutron and gamma spectrum concurrently. This is not possible for the smaller detectors because of their low detection efficiency for photons with energy over 5 MeV.

The output of both codes includes:

- Neutron (resp. gamma) spectrum in numeric form with energetic step either 0.05, 0.1, or 0.2 MeV.
- Neutron flux density in wide energetic groups.
- The above mentioned results are characterized by standard (resp. extended) type A uncertainties.
- Graphical representation in selected scale(s) (e.g. lin-lin, log-lin etc.).

Type B uncertainties are not part of the output since they are difficult to determine. They can be derived from measurement results in referential fields or from benchmarks. In both cases the experimental results are compared with computation of e.g. transport of a mixed field in precisely defined geometry and other conditions of computation and experiment [15]. From the comparison we can draw conclusions about the model, nuclear data used, measuring device operation, and evaluation of experimental data.

The above described spectrometric system has been successfully used e.g. in experiments to quantify the protective properties of building materials and both military and civil objects and vehicles against penetration of neutron and photon radiation [16]. Another application area is acquisition of data about energetic and spatial distribution of a mixed field in models of segment of energetic reactors of type WWER 440 and WWER 1000. The data serves as a basis for evaluation of radiation embrittlement of reactor pressure vessel. The experiments take place in experimental reactor LR-0 in NRI Rez; the model of a segment of WWER is built in its vessel [17, 18].

In addition, the research of neutron sources controlled by accelerator was interesting, too. Such sources head towards solution to the nuclear waste problem using subcritical reactors [19].

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