

# NUCLEAR CONSTANTS DATABASE FOR FUEL ISOTOPE CHANGE ESTIMATION

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Description of database and client program developed by the authors and designed to store, process and extract nuclear constants used in calculations of nuclear fuel isotope changes is presented. On the basis of the designed database, a comprehensive program was developed. The program allows calculating the change in nuclear concentration and activity of fuel isotopes during irradiation and exposure.

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## INTRODUCTION

One of the most important aspects of nuclear power is the control of the state and changes in the isotopic composition of nuclear fuel. At present, the assessment of the fuel state is required in justifying the safety of nuclear power plants, marine facilities, as well as SNF (spent nuclear fuel) storages [1]. During this process it is necessary to take into account many factors: fuel type, reactor core composition, heat power, fuel recharging regime and so on, which become even more crucial in modeling of long-lived radioactive waste transmutation [2 - 4]. Effective transmutation, in turn, is impossible without preliminary optimization [5], aimed at determining the initial fuel loading, moments of fuel recharging and the reactor control mode. The existing nowadays commercial programs (for example, ORIGEN [6], etc.) allow to determine the concentrations change of fuel isotopes in variant calculations with a sufficiently high accuracy, however they are not designed for solving optimization problems. The purpose of this work is to develop a software package and nuclear constants database for isotope fuel change estimating, and which, in particular, can solve the optimization problem for transmutation process in various facilities.

## 1. FUEL ISOTOPE CHANGE

The time variation in atomic number density ( $N_i$ ) of a target nuclide ( $i$ ) can be expressed as the following differential equation [7]:

$$\frac{dN^i}{dt} = \sum_{j \neq i} f^{j \rightarrow i} \lambda^j N^j + \sum_{k \neq i} \sum_x g_x^{k \rightarrow i} N^k \langle \sigma_x^k \phi \rangle + \sum_l \gamma^{l \rightarrow i} F^l - (\lambda^i + \langle \sigma_a^i \phi \rangle) N^i, \quad (1)$$

where the first term on the right-hand side is the production rate of nuclide  $i$  due to radioactive decay of another nuclide  $j$  on the burnup chain.  $\lambda^j$  is the decay constant of nuclide  $j$  and  $f^{j \rightarrow i}$  is the probability of decay to nuclide  $i$ . The second term is the production rate of nuclide  $i$  in the nuclear reaction  $x$  of another nuclide  $k$ .  $g_x^{k \rightarrow i}$  is the probability of transmutation into nuclide  $i$  for nuclear reaction  $x$  of nuclide  $k$ . The third term is for the production of FPs.  $F^l$  is the fission rate of heavy nuclide  $l$  and  $\gamma^{l \rightarrow i}$  is the yield fraction of nuclide  $i$  for the fission reaction. The last term is the loss rate of nu-

clide  $i$  due to radioactive decay and absorption reactions,  $\langle \sigma_x^k \phi \rangle$  – is defined by the following relation:

$$\langle \sigma_x^k \phi \rangle = \frac{E_{\max}}{E_{\min}} \int \sigma_x^k(E) \phi(E) dE = \sum_{i=1}^n \sigma_x^k(E_i) \phi(E_i) \Delta E_i. \quad (2)$$

Here  $\phi(E_i)$  – neutron flux, normalized to the reactor heat power. Neutron flux is calculated via solving the neutron transport equation in the lattice in multi-group diffusion approximation using the program code MDSR [8].

The matrix of the system (1) (transition matrix) is formed on the basis of the so-called burnup chain, both for actinides and fission products (an example is shown in Fig. 1).

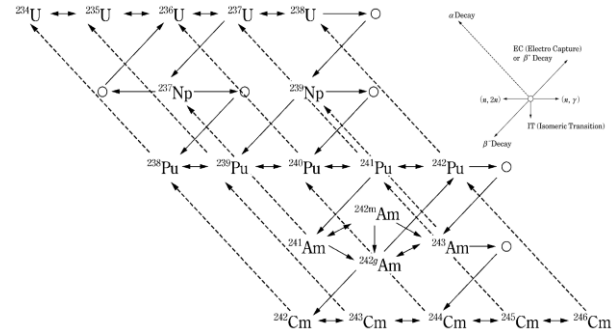


Fig. 1. An example burnup chain of heavy metals [7]

Using equation (1), it is possible to calculate both the isotope change, the quantity of fission products and actinides during the reactor operation and at the time of reactor shutdown, as well as spent fuel isotope evolution (in this case  $\langle \sigma_x^k \phi \rangle = 0$  and  $F^l = 0$ ).

Applying (1) to all nuclides including fission products on the burnup chain gives simultaneous differential equations (burnup equations) corresponding to the number of considered nuclides. In view of the transition matrix structure ways to solve the burnup equations (1) include analytical Bateman method [9] and the matrix exponential method [10].

## 2. EVALUATED NUCLEAR DATA FILES

Group nuclear constants  $\sigma_x^k(E_i)$  in (2), as well as coefficients, characterizing radioactive transitions in (1) are the public data, stored in so called evaluated nuclear data files which includes cross sections uniquely-determined in the whole range of neutron energy on the basis of fragmentally measured and/or theoretically cal-

culated parameters, radioactive decays etc. of more than 400 nuclides [7, 11]. The most used evaluated nuclear data files are JENDL [12], ENDF/B [13], JEFF [14].

The evaluated nuclear data from anywhere in the world are described and stored in the same way in 80-column text format that provides information in a block structure. The format has been changed according to advances in nuclear data and the current latest format is called ENDF-6 [15].

The ideology of evaluated nuclear data files formation was formed at a time when the possibilities of computer technology were significantly limited, and the reliability of its work left much to be desired. Therefore, a number of principles have been implemented in these files format, that now appear as something of an atavism. A fragment of the ENDF-6 file is shown in Fig. 2. As can be seen from the figure, working with such files is quite difficult.

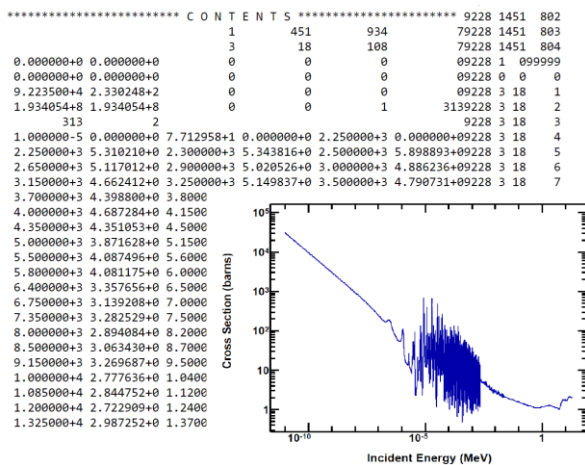


Fig. 2. Example of  $^{235}\text{U}$  fission cross section stored in ENDF/B-VII.1 (Right bottom figure: plot of the cross section) [16]

### 3. NUCLEAR CONSTANTS DATABASE

For the convenient and universal use of nuclear data, a relational database (under management of MS SQL Server) and associated client application (MS C #) (Fig. 3) were designed.

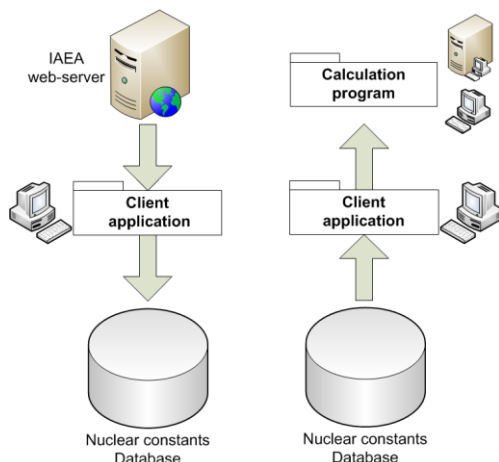


Fig. 3. Modes of database communication with client and calculation programs

Client application operates in two modes: to write and read data. In the data writing mode, text files for all isotopes of the selected library are downloaded in the

ENDF-6 format from the IAEA nuclear data section server [16]. After then they are read and the required data are extracted followed by the subsequent recording to the database. It should be noted that the database structure dynamically expands during data downloading for each subsequent isotope. In read mode, the client program executes a request to extract data on the reactions cross sections, radioactive decays, etc., required to perform calculations. After then it transforms data to the form used by calculation program. The communication between database and client application is carried out using stored procedures.

Fig. 4 shows a fragment of the nuclear constants database structure.

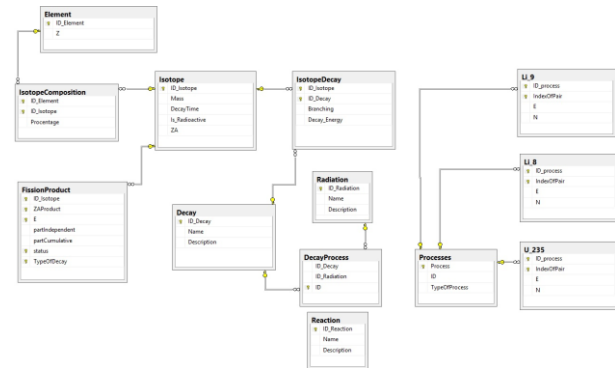


Fig. 4. ER-model of nuclear constants database

The special feature of the developed client program is that it can work independently from the calculation code, as a stand-alone software product designed to visualize and display data in a user-friendly form (Fig. 5).



Fig. 5. User interface of the client program for communication with the database

The main task of the client program is to restore the burnup chains (see Fig. 1) of considered isotopes in order to form the transition matrix of the system (1), as well as to select the most significant isotopes in the context of the problem being solved for the dimension reduction. The choice depends on the objectives of transmutation (fission products or actinides), radiotoxicity and lifetime of isotopes, and also the campaign period.

### 4. DEPLETION AND BUILDUP TESTS

Using the bundle of the developed nuclear constants database and the client program, as well as the calculation module for solving the system (1), the processes of fuel depletion and fission products buildup for the research reactor U-3 [17] were simulated. The changes in the isotopes total activity in the U-3 core after operation in the following regimes are analyzed:

- Regime 1. Heat power (W) = 50 kW, operation time (Tk) 100 hours (energy-producing 5 MW·hour);
- Regime 2. Heat power (W) = 15 kW, operation time (Tk) 1000 hours (energy-producing 15 MW·hour);
- Regime 3. Storing.

Dependences of the reactor U-3 core activity in different operation regimes on the time after reactor shutdown are shown in Fig. 6.

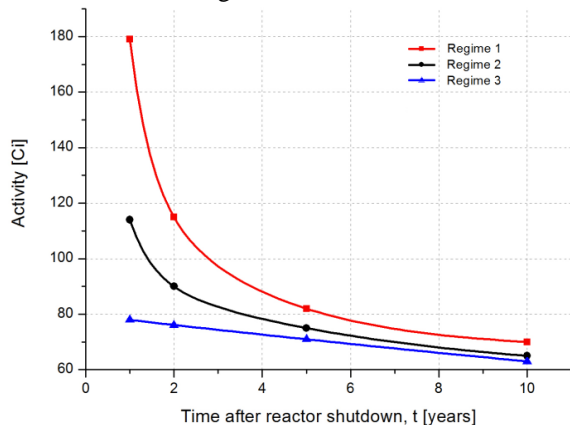


Fig. 6. Dependences of the reactor U-3 core activity on the time after reactor shutdown

Also, isotopes which give the largest contribution to the total activity of the fuel at different times were identified. Table 1 shows data on the most significant isotopes in the reactor first operating mode immediately after the reactor shutdown, and Table 2 – after 10 years of exposure.

Table 1

Isotopes that determine the activity of the reactor core after operation in mode 1, immediately after reactor shutdown

t = 0 years		
Isotope name	Activity [Ci]	% from the total reactor core activity
U-239	3830	3.48
I-134	3300	3.00
Np-239	3230	2.93
Cs-138	2810	2.55
I-133	2760	2.51
Ba-139	2710	2.46
Te-134	2690	2.44
Xe-135	2680	2.43
I-135	2680	2.43
Y-92	2560	2.33
Sr-91	2530	2.30
La-142	2510	2.28
La-141	2490	2.26
Sr-92	2470	2.24
Nb-97	2390	2.17
Zr-97	2370	2.15
Y-94	2350	2.13
Nb-97M	2250	2.04
Ce-143	2230	2.03
Tc-101	2120	1.93
Xe-138	2040	1.85
Ba-141	2010	1.83
Y-95	1920	1.74
La-143	1920	1.74

Table 2

Isotopes that determine the activity of the reactor core after operation in mode 1 10 years after the reactor shutdown

t = 10 years		
Isotope name	Activity [Ci]	% from the total reactor core activity
Cs-137	16.7	25.63
Ba-137M	15.8	24.25
Sr-90	15.6	23.94
Y-90	15.6	23.94

The obtained results are consistent with the measurements results. This fact confirms the correctness of the developed software.

## CONCLUSIONS

Description of the nuclear constants database and a client application linking it to the calculation program are presented in this paper. Filling in the database comes from the updating public archive of the IAEA nuclear data section, which guarantees the reliability of the data used in the calculations. A special feature of the developed software is the possibility of reducing the burnup chains and the number of considered isotopes. This feature makes it possible to use the complex for optimization. The work of the software package and database is illustrated in the calculation tests for the research reactor U-3. The obtained results are consistent with the measurements.

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### **БАЗА ДАННЫХ ЯДЕРНЫХ КОНСТАНТ ДЛЯ ОЦЕНКИ ИЗМЕНЕНИЯ ИЗОТОПНОГО СОСТАВА ТОПЛИВА**

*А.Г. Головкина, А.Д. Лоскутова, Д.А. Овсянников*

Представлено описание разработанной авторами базы данных и клиентской программы, предназначенных для хранения, обработки и извлечения ядерных констант, используемых при расчетах динамики изменения изотопного состава ядерного топлива. На основе созданной базы данных была разработана комплексная программа, позволяющая рассчитывать изменение ядерной концентрации и активности изотопов топливной композиции в процессе облучения и выдержки.

### **БАЗА ДАНИХ ЯДЕРНИХ КОНСТАНТ ДЛЯ ОЦІНКИ ЗМІНИ ІЗОТОПНОГО СКЛАДУ ПАЛИВА**

*А.Г. Головкина, А.Д. Лоскутова, Д.А. Овсянников*

Представлено опис розробленої авторами бази даних і клієнтської програми, призначених для зберігання, обробки та вилучення ядерних констант, використовуваних при розрахунках динаміки зміни изотопного складу ядерного палива. На основі створеної бази даних була розроблена комплексна програма, що дозволяє розраховувати зміну ядерної концентрації і активності ізотопів паливної композиції в процесі опромінення і витримки.