Mathematical modelling of heat production in deep geological repository of high-level nuclear waste

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Abstract

Waste produced by nuclear industry requires special handling. Currently, there is a research taking place, focused at possibilities of nuclear waste storage in deep geological repositories, hosted in stable geological environment. The high-level nuclear waste produces significant ammount of heat for a long time, which can affect either environment outside of or within the repository in a negative way. Therefore to reduce risks, it is desirable to know the principles of such heat production, which can be achieved using mathematical modeling. This thesis comes up with a general model of heat production-time dependency, dependable on initial composition of the waste. To be able to model real situations, output of this thesis needs to be utilized in an IT solution.

Keywords: *High-level waste; decay constant; Q-value; heat production*

Introduction and aim formulation

Nuclear energetics is a growing industry in a worldwide scale [1]. Just like any other industry, it produces waste. Such waste is not big in volume, however, has to be treated as hazardous in special kind of way. Nowadays, companies are making efforts to design a long-term repository for nuclear waste [2]. For safety-at-lowest-maintanance reasons, these repositories are planned to be situated underground in stable geological environment. Nuclear waste remains hazardous even after a long time. To be designed properly, in order to prevent leakage, and to minimize environmental impact, it's essential to know as much about the waste's features development in time as possible. One of the key features, directly involving environment of either the repository itself or the host geological formation, is heat production of the waste. Once the heat production, dependable on mass and isotopic composition of the waste, is known, we are a step closer to designing the repository as a safe, low impact structure, without over or undersized components.

Material and methods

In nature, the way elements decay into other elements can be described with probability. For example, if we had a sample of one microgram ^{238}U, containing about 2,5 x 10^{18} nuclei, by experimental measuring we could specify, that every second 12 nuclei will decay, yet there is no way to determine, which nucleus will decay next. The likelihood of decay is the same with any nucleus. Mathematicaly, this can be described by integrated law of nuclear decay:

$$N = N_0 \cdot e^{-\lambda t} \quad \text{[I.]}$$

where N is actual number of nuclei, N_0 the original count of nuclei and λ is decay constant. Energy released during this process is given by Einsten's mass-energy relation:

$$E = \Delta m \cdot c^2 \quad \text{[II.]}$$

Energy is released in the form of kinetic energy of daughter products, but transforms into heat eventualy in the repository or in it's near vicinity. Daugter products can undergo further decay. We therefore have to deal with a chain of linear differential equations, each of which being an initial condition of the following equation. The basic idea of the model is then:

$$P(t) = \sum_i P_i = -\sum_i Q_i \cdot \lambda_i \cdot n_i \quad \text{[III.]}$$

This equation basically says, that the total heating performance (P(t)) is equal to the sum of heating performances of all the decaying nuclei contained in modeled sample, which are represented by the decay velocity, obtained as a derivative of the law of nuclear decay ($-\lambda_i \cdot n_i$), multiplied by respective Q-value (Q_i). The minus sign indicates that the heat is produced, not consumed, consitently with the Law of nuclear decay. [3]

Results and discussion

To determine the velocities of respective daughter generation's decay, we need to write down a system of differential equations of the form:

$$\frac{dn_i}{dt} = \lambda_{i-1} \cdot n_{i-1} - \lambda_i \cdot n_i \quad \text{[IV.]}$$

The first term on right hand side of [IV.] is the contribution of previous generation's decay, the other represents the decay of i-th generation itself. Let us assume, that our decay chain contains *J* generations. To calculate respective velocities explicitely, we need to find eigenfunctions of a following linear operator:

$$\begin{pmatrix} \frac{dn_0}{dt} & \frac{dn_1}{dt} & \cdots & \frac{dn_J}{dt} \end{pmatrix} = \begin{pmatrix} n_0 & n_1 & \cdots & n_J \end{pmatrix} \begin{pmatrix} -\lambda_0 & \lambda_0 & 0 & \dots & 0 & 0 \\ 0 & -\lambda_1 & \lambda_1 & & 0 & 0 \\ 0 & 0 & -\lambda_2 & & 0 & 0 \\ \vdots & & & \ddots & \lambda_{J-2} & 0 \\ 0 & 0 & 0 & 0 & -\lambda_{J-1} & \lambda_{J-1} \\ 0 & 0 & 0 & 0 & 0 & -\lambda_J \end{pmatrix} \quad \text{[V.]}$$

This system is homogenous. It can be solved by finding it's eigenvalues and eigenvectors with premise, that the solution is made of exponential functions. Explicite solution for i-th generation is then:

$$n_i(t) = N_0\left(\prod_{j=0}^{i-1}\lambda_j\right)\sum_{j=0}^{i-1}\frac{e^{-\lambda_j \cdot t} - e^{-\lambda_i \cdot t}}{\prod_{k=0,k\neq j}^{i}(\lambda_k - \lambda_j)}$$

[VI.]

Therefore, for heating performance-time dependency of i-th generation we get:

$$P_i(t) = -Q_i \cdot \lambda_i \cdot n_i = -N_0 Q_i\left(\prod_{j=0}^{i}\lambda_j\right)\sum_{j=0}^{i-1}\frac{e^{-\lambda_j \cdot t} - e^{-\lambda_i \cdot t}}{\prod_{k=0,k\neq j}^{i}(\lambda_k - \lambda_j)}$$

[VI.]

And finaly, for the heating performance-time dependency of the whole decay chain:

$$P(t) = \sum_{i=0}^{J} P_i = -N_0 \sum_{i=0}^{J} Q_i\left(\prod_{j=0}^{i}\lambda_j\right)\sum_{j=0}^{i-1}\frac{e^{-\lambda_j \cdot t} - e^{-\lambda_i \cdot t}}{\prod_{k=0,k\neq j}^{i}(\lambda_k - \lambda_j)}$$

[VII.]

Last issue is determination of the zero-generation initial nuclei count. This can be achieved in rather intuitive way, only using the weight-percentages w_l of components of the modelled system in time t=0 and it's total mass m. Initial nuclei count of l-th component is then:

$$N_{0,l} = \frac{w_l \cdot m}{M_l} \cdot N_A$$

[VIII.]

where N_A is the Avogadro constant and M_l the molar weight of zero-generation isotope.

By substituting [VIII.] into [VII.], we get the total solution of the problem:

$$P(t) = m \cdot N_A \sum_{l=1}^{N}\frac{w_l}{M_l} \cdot \left[\sum_{i=0}^{J} Q_i\left(\prod_{j=0}^{i}\lambda_j\right)\sum_{j=0}^{i-1}\frac{e^{-\lambda_j \cdot t} - e^{-\lambda_i \cdot t}}{\prod_{k=0,k\neq j}^{i}(\lambda_k - \lambda_j)}\right]$$

[IX.]

This model is based on presupposition, that all nuclear reactions (decays) are naturally driven. It does not involve neutron - invoked reactions, such as those occuring in reactor. Judging from the fact, that such induced reactions do need to be actively maintained during nuclear power generation, and soon enough vanish once the material is removed from the reactor [2, 4], this premise is real. Model also counts on the fact, that every generation decays in one particular way, thus it does not model the situation, when an isotope can undergo alpha or beta decay with respective probabilities. Considering that in such cases the ratio of the lower probability to the higher is very low, uncertainity caused by this is low enough when computing the model using only the more probable decay. If required, this can be fixed by breaking the influenced daughter generation into two separate decay sequences, each multiplied with respective probability factor. Last situation not computable with this formula is, when two decay constants within a decay chain have the exactly same value (problem with dividing by zero). However, this situation does not have been encountered in any of decay sequences, determined by Evaluated Nuclear Data Files library. It is worth to also mention that [VI.] and [VII.], which are, in the end, part of [IX.], contain 2^{i-1}

fractions with exponential numerators. If we assume a decay chain of 15 generations, the last one would be described by more than 16000 quite non-elementary fractions. It is therefore rather unpractical to use [IX.] without a proper computer program.

Conclusion

To be able to model heat production of high-level nuclear waste, we can employ law of nuclear decay and Q-values to get heating performance-time dependence. Once we obtain decay velocities by solving a system of linear differential equations, we need to multiply respective decay-velocity functions with their respective Q-values. Further, we need to determine initial count of each decay chain's zero-generation. Put together, we obtain the time dependence of heating performance of the modelled waste:

$$P(t) = m \cdot N_A \sum_{l=1}^{N} \frac{w_l}{M_l} \cdot \left[\sum_{i=0}^{J} Q_i \left(\prod_{j=0}^{i} \lambda_j \right) \sum_{j=0}^{i-1} \frac{e^{-\lambda_j \cdot t} - e^{-\lambda_i \cdot t}}{\prod_{k=0, k \neq j}^{i} (\lambda_k - \lambda_j)} \right] \qquad \text{[IX.]}$$

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