Supporting Information

for

"Inventories of Short-Lived Fission Gas Nuclides in Nuclear Reactors"

Yu Wang, Jianzhu Cao, Feng Xie * and Fu Li

Institute of Nuclear and New Energy Technology, Collaborative Innovation Center of Advanced Nuclear Energy Technology, Key Laboratory of Advanced Reactor Engineering and Safety of Ministry of Education, Tsinghua University, Beijing 100084, China

* Correspondence: fxie@tsinghua.edu.cn

Equations (2)-(4) are the simplification of Equation (1) and justified in the paper. Equations (5)-(14) and Equation (23) are simplified from the analytic solution of Equation (1) for the short-lived fission gas nuclides, whose derivation are added as the supporting information below. Equations (15)-(22) are the fitting formula and the fitting results for HTR-10 core with the fitting data calculated by KORIGEN in the Figures 6 and 7. Equations (24)-(27) are justified in the paper based on Equation (23).

1. Point depletion burnup equation

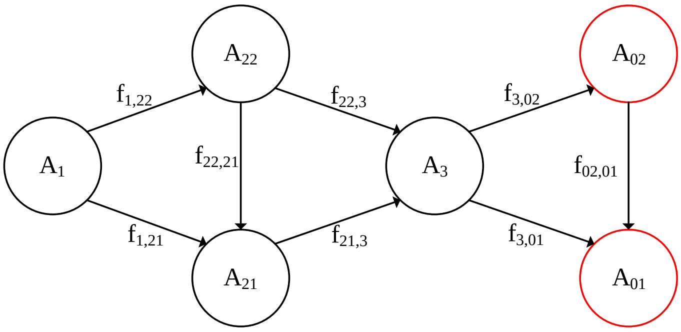
The general point-depletion burnup equation is as follows:

$$\frac{dN_i}{dt} = \sum_{j=1}^{n_j} l_{ij}\lambda_j N_j + \phi\sum_{j=1}^{N} f_{ij}\sigma_j N_j - (\lambda_i + \phi\sigma_{a,i})N_i, \qquad i = 1,2,\dots,N \tag{S1}$$

where N_i represents the atom numbers of radionuclide i, N_j is the amount of precursor nuclide j or fissionable nuclides j, n_j is the total number of precursor nuclides i, N is the number of fissionable nuclides, λ_i is the decay constant of radionuclide i [s^{-1}], $\sigma_{a,i}$ is the spectrally averaged neutron absorption cross-section [cm^2], σ_j is the spectrally averaged cross-section that yields the nuclide i [cm^2], l_{ij} is the fraction from radionuclide j decay into nuclide i, f_{ij} is the fraction from nuclides j to radionuclide i, especially the fission yields from fissionable nuclides j to radionuclide i, and ϕ is the neutron flux averaged by space and energy [cm^{-2} s^{-1}].

1.1 Decay chain for model A

1.1.1 Decay chain for Sub-mode A_0



a) Decay chain for mode A

Figure S1. General mode A for the decay chain

$A_{f,j}$ is defined as the number of nuclides j from the nuclear fission reaction per unit time, which is included in the second item, $\phi\sum_{j=1}^{N} f_{ij}\sigma_j N_j$, on the right-hand side of the Equation (S1).

$$A_{f,j} = \sum_i Y_{i,j}\sigma_{f,i}\phi N_i \quad i = U5, U8, Pu9, Pu1 \tag{S2}$$

The following conditions were applied for the above equations:

- The (n, γ) neutron absorption reaction was only considered for ^{135}Xe and ^{133}Xe;
- ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu were considered for fissionable nuclides; and
- All fission gas nuclides were assumed to be in equilibrium, where $\frac{dN_i}{dt} = 0, i = 1,21,22,3,01$, or 02.

The (n, γ) neutron absorption reaction was only considered for ^{135}Xe and ^{133}Xe, which means nuclide i is not from the neutron absorption of other non-fissile nuclides in our consideration. In the second item, $\phi\sum_{j=1}^{N} f_{ij}\sigma_j N_j$, on the right-hand side of the Equation (S1) only embracing the fission fissile nuclides. ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu were considered for fissionable nuclides. Therefore, for nuclide j, $A_{f,j} = \phi\sum_{j=1}^{N} f_{ij}\sigma_j N_j$. The first item on the right-side of the Equation (S1) depends on decay chain such as the figure "Decay chain for the mode

A″ above. For each nuclide in the figure, the equation for nuclide *i* reflects that the variation of atom numbers of radionuclide *i* is equal to the birth rate minus remove rate as follows:

$$\frac{dN_{01}}{dt} = -(\lambda_{01} + \sigma_{a,01}\phi)N_{01} + (f_{02,01}\lambda_{02}N_{02} + f_{3,01}\lambda_3 N_3) + A_{f,01} \tag{S3}$$

$$\frac{dN_{02}}{dt} = -\lambda_{02}N_{02} + f_{3,02}\lambda_3 N_3 + A_{f,02} \tag{S4}$$

$$\frac{dN_3}{dt} = -\lambda_3 N_3 + f_{21,3}\lambda_{21}N_{21} + f_{22,3}\lambda_{22}N_{22} + A_{f,3} \tag{S5}$$

$$\frac{dN_{21}}{dt} = -\lambda_{21}N_{21} + f_{1,21}\lambda_1 N_1 + f_{22,21}\lambda_{22}N_{22} + A_{f,21} \tag{S6}$$

$$\frac{dN_{22}}{dt} = -\lambda_{22}N_{22} + f_{1,22}\lambda_1 N_1 + A_{f,22} \tag{S7}$$

$$\frac{dN_1}{dt} = -\lambda_1 N_1 + A_{f,1} \tag{S8}$$

All fission gas nuclides were assumed to be in equilibrium, where $\frac{\mathrm{dN_i}}{\mathrm{dt}} = 0, \mathrm{i} =$ 1,21,22,3,01, or 02. Equations (S3)-(S8) become as follows:

$$0 = -(\lambda_{01} + \sigma_{a,01}\phi)N_{01} + (f_{02,01}\lambda_{02}N_{02} + f_{3,01}\lambda_3 N_3) + A_{f,01} \tag{S9}$$

$$0 = -\lambda_{02}N_{02} + f_{3,02}\lambda_3 N_3 + A_{f,02} \tag{S10}$$

$$0 = -\lambda_3 N_3 + f_{21,3}\lambda_{21}N_{21} + f_{22,3}\lambda_{22}N_{22} + A_{f,3} \tag{S11}$$

$$0 = -\lambda_{21}N_{21} + f_{1,21}\lambda_1 N_1 + f_{22,21}\lambda_{22}N_{22} + A_{f,21} \tag{S12}$$

$$0 = -\lambda_{22}N_{22} + f_{1,22}\lambda_1 N_1 + A_{f,22} \tag{S13}$$

$$0 = -\lambda_1 N_1 + A_{f,1} \tag{S14}$$

Solving above equation system, analytical results can easily get as follows, the Equations (S15) and (S16):

$$I_{02} = \lambda_{02}N_{02} = f_{3,02}(A_{f,1} + A_{f,21} + A_{f,22} + A_{f,3}) + A_{f,02} \tag{S15}$$

$$I_{01} = \lambda_{01}N_{01} = (A_{f,1} + A_{f,21} + A_{f,22} + A_{f,3} + A_{f,02} + A_{f,01})\frac{\lambda_{01}}{\lambda_{01} + \sigma_{a,01}\phi} \tag{S16}$$

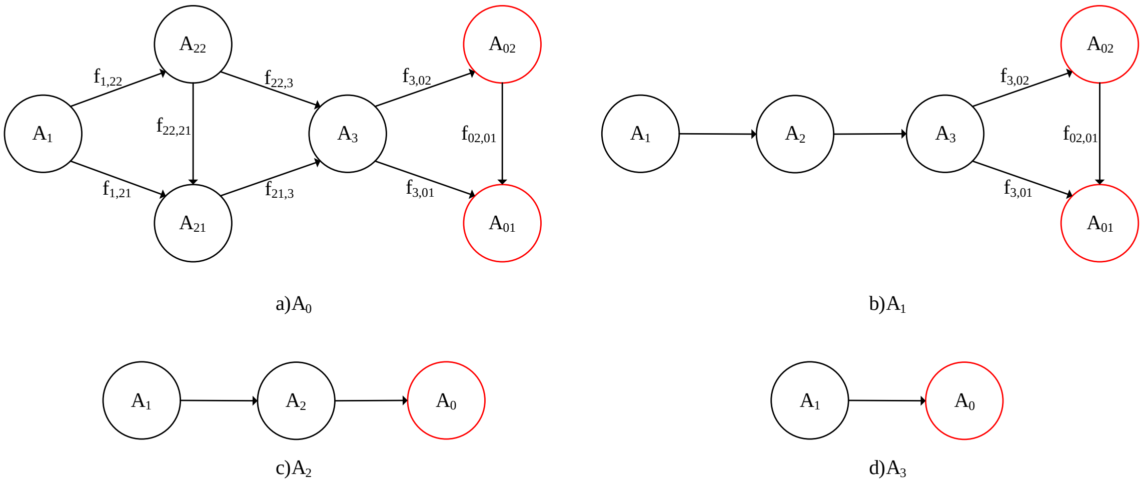


Figure S2. Sub-modes of general mode A for the decay chain of the fission gas nuclide

1.1.2 Decay chain for Sub-mode A_1

Similar equation system can be obtained from the Figure S2 b).

$$\frac{dN_{01}}{dt} = -(\lambda_{01} + \sigma_{n,01}\phi)N_{01} + (\lambda_{02}N_{02} + f_{3,01}\lambda_3 N_3) + A_{f,01} = 0 \quad \text{(S17)}$$

$$\frac{dN_{02}}{dt} = -\lambda_{02}N_{02} + f_{3,02}\lambda_3 N_3 + A_{f,02} = 0 \quad \text{(S18)}$$

$$\frac{dN_3}{dt} = -\lambda_3 N_3 + \lambda_2 N_2 + A_{f,3} = 0 \quad \text{(S19)}$$

$$\frac{dN_2}{dt} = -\lambda_2 N_2 + \lambda_1 N_1 + A_{f,2} = 0 \quad \text{(S20)}$$

$$\frac{dN_1}{dt} = -\lambda_1 N_1 + A_{f,1} = 0 \quad \text{(S21)}$$

Analytical results can be easily derived as follows in the Table 2 in the paper:

$$I_{01} = (A_{f,1} + A_{f,2} + A_{f,3} + A_{f,02} + A_{f,01})\frac{\lambda_{01}}{\lambda_{01} + \sigma_{a,01}\phi} \quad \text{(S22)}$$

$$I_{02} = f_{3,02}(A_{f,1} + A_{f,2} + A_{f,3}) + A_{f,02} \quad \text{(S23)}$$

1.1.3 Decay chain for Sub-mode A_2

Similar equation system can be obtained from the Figure S2 c).

$$\frac{dN_0}{dt} = -\lambda_0 N_0 + \lambda_2 N_2 + A_{f,0} = 0 \quad \text{(S24)}$$

$$\frac{dN_2}{dt} = -\lambda_2 N_2 + \lambda_1 N_1 + A_{f,2} = 0 \quad \text{(S25)}$$

$$\frac{dN_1}{dt} = -\lambda_1 N_1 + A_{f,1} = 0 \quad \text{(S26)}$$

Analytical results can be easily derived as follows in the Table 2 in the paper:

$$I_0 = f_{2,0}(f_{1,2}A_{f,1} + A_{f,2}) + A_{f,0} \tag{S27}$$

1.1.4 Decay chain for Sub-mode A3

Similar equation system can be obtained from the Figure S2 d).

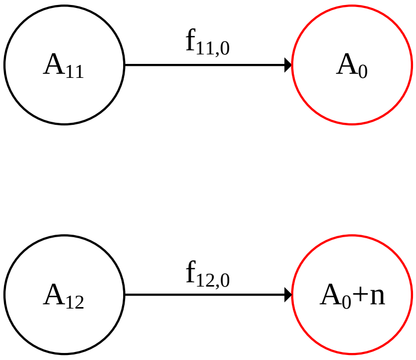
$$\frac{dN_0}{dt} = -\lambda_0 N_0 + \lambda_1 N_1 + A_{f,0} \tag{S28}$$

$$\frac{dN_1}{dt} = -\lambda_1 N_1 + A_{f,1} \tag{S29}$$

Analytical results can be easily derived as follows in the Table 2 in the paper:

$$I_0 = f_{1,0}A_{f,1} + A_{f,0} \tag{S30}$$

1.2 Decay chain for model B



a) Decay chain for mode B

Figure S3. General mode B for the decay chain

Similar equation system can be obtained from the Figure S3.

$$\frac{dN_0}{dt} = -\lambda_0 N_0 + \left(f_{11,0}\lambda_{11}N_{11} + f_{12,0}\lambda_{12}N_{12}\right) + A_{f,0} \tag{S31}$$

$$\frac{dN_{11}}{dt} = -\lambda_{11}N_{11} + A_{f,11} \tag{S32}$$

$$\frac{dN_{12}}{dt} = -\lambda_{12}N_{12} + A_{f,12} \tag{S33}$$

Analytical results can be easily derived as follows in the Table 2 in the paper:

$$I_0 = f_{11,0}A_{f,11} + f_{12,0}A_{f,12} + A_{f,0} \tag{S34}$$

Equation (S35) can be easily derived because of I_0, I_{01} and I_{02} in all decay mode in the Table 2 in the paper.

$$I_i = g\left(A_{f,j}\right) = \sum_j \alpha_{j,i}A_{f,j} \tag{S35}$$

$$I_{01} = A_f(\phi)\frac{\lambda_{01}}{\lambda_{01}+\sigma_{a,01}\phi} \tag{S36}$$

Equation (S36) can be easily derived from Equation (S16) as follows:

$$I_{01} = \lambda_{01} N_{01} = \left(A_{f,1} + A_{f,21} + A_{f,22} + A_{f,3} + A_{f,02} + A_{f,01}\right) \frac{\lambda_{01}}{\lambda_{01} + \sigma_{a,01}\phi} = \left(\sum_i Y_{i,1}\sigma_{f,i}\phi N_i + \sum_i Y_{i,21}\sigma_{f,i}\phi N_i + \sum_i Y_{i,22}\sigma_{f,i}\phi N_i + \sum_i Y_{i,02}\sigma_{f,i}\phi N_i + \sum_i Y_{i,01}\sigma_{f,i}\phi N_i\right) \frac{\lambda_{01}}{\lambda_{01} + \sigma_{a,01}\phi} = A_f(\phi) \frac{\lambda_{01}}{\lambda_{01} + \sigma_{a,01}\phi} \quad \text{(S37)}$$

$$A_f(\phi) = \left(\sum_i Y_{i,1}\sigma_{f,i}\phi N_i + \sum_i Y_{i,21}\sigma_{f,i}\phi N_i + \sum_i Y_{i,22}\sigma_{f,i}\phi N_i + \sum_i Y_{i,02}\sigma_{f,i}\phi N_i + \sum_i Y_{i,01}\sigma_{f,i}\phi N_i\right) = \phi\left(\sum_i Y_{i,1}\sigma_{f,i} N_i + \sum_i Y_{i,21}\sigma_{f,i} N_i + \sum_i Y_{i,22}\sigma_{f,i} N_i + \sum_i Y_{i,02}\sigma_{f,i} N_i + \sum_i Y_{i,01}\sigma_{f,i} N_i\right) \quad \text{(S38)}$$

where $i = U5, U8, Pu9, Pu1$.