Mathematical Expressions for the Fractional Release of a Fission Product from an HTR Nuclear Fuel Element

Young Min Kim<sup>1</sup>, Tae Hoon Lee, and Chang Keun Jo Korea Atomic Energy Research Institute 111, Daedeok-daero 989beon-gil, Yuseong-gu, Daejeon, 34057, Korea <sup>1</sup> Corresponding author: nymkim@kaeri.re.kr

# **Objectives**

The quantity called fractional release (FR) (or release fraction) is used as a measure quantifying the fission product (FP) release in many high temperature reactor (HTR) fuel performance analysis code.



This study describes the mathematical expressions of the FP releases from an HTR fuel element, and the analytical forms of FRs for the radioactive and stable isotopes diffusing out of a spherical particle.

### **Fractional Release Formulae**

#### **Radioactive fission product**

#### **Stable fission product**

$C = \text{concentration (atoms/m^3)}, \dot{B} = \text{volumetric birth rate (atoms/(m^3 s))}, \lambda = \text{decay constant (s^{-1})}, D = \text{diffusion coefficient (m^2/s)}, r = \text{radial coordinate (m)}, t = \text{time (s)}, t = ti$			$C = \text{concentration (atoms/m^3)}, \dot{B} = \text{volumetric birth rate (atoms/(m^3 s))}, \lambda = \text{decay constant (s^-1)}, D = \text{diffusion coefficient (m^2/s)}, r = \text{radial coordinate (m)}, t = \text{time (s^-1)}, t =$		
$z = 0$ for a slab, 1 for a cylinder, 2 for a sphere, $J = \text{mass current}$ , $(\text{atoms}/(\text{m}^2 \text{ s}))$ , $C^{(0)} = \text{initial concentration}$ $(\text{atoms}/\text{m}^3)$ , $C_V = \int_V C dV = \text{amount in a volume (atoms)}$ ,			$z = 0$ for a slab, 1 for a cylinder, 2 for a sphere, $J = \text{mass current}$ , $(\text{atoms}/(\text{m}^2 \text{ s}))$ , $C^{(0)} = \text{initial concentration}$ $(\text{atoms}/\text{m}^3)$ , $C_V = \int_V C dV = \text{amount in a volume}$ $(\text{atoms}/\text{m}^2 \text{ s})$		
$\dot{R}_V$ = release rate (atoms/s), $\dot{B}_V = \int_V \dot{B} dV$ = birth rate (atoms/s), $V$ = volume (m <sup>3</sup> ), $R_V$ = amount released (atoms), $B_V$ = amount generated (atoms),			$\dot{R}_V$ = release rate (atoms/s), $\dot{B}_V = \int_V \dot{B} dV$ = birth rate (atoms/s), $V$ = volume (m <sup>3</sup> ), $R_V$ = amount released (atoms), $B_V$ = amount generated (atoms),		
$A_s = \text{surface area } (\text{m}^2), \ \mu = \lambda a^2 / D, \ \tau(t) = \int_0^t [D(r, x) / a^2] dx, \ a = \text{radial coordinate of the outermost location } (\text{m}), \ F_{irr}^{(e)} = \text{fractional release at the end of irradiation.}$			$A_s = \text{surface area } (\text{m}^2), \ \mu = \lambda a^2 / D, \ \tau(t) = \int_0^t [D(r,x)/a^2] dx, \ a = \text{radial coordinate of the outermost location } (\text{m}), \ F_{irr}^{(e)} = \text{fractional release at the end of irradiation.}$		
Phases	Quantities	Fractional release formulae for a sphere with a constant $D$ and a constant $\dot{B}$	Phases	Quantities	Fractional release formulae for a sphere with a constant D and a constant $\dot{B}$
Irradiation phase: $\frac{\partial C}{\partial t} = \dot{B} - \lambda C + \frac{1}{r^{z}} \frac{\partial}{\partial r} \left( r^{z} D \frac{\partial C}{\partial r} \right)$ $C(a,t) = C(r,0) = 0$ $J(0,t) = 0$ $\frac{dC_{V}}{dt} = \dot{B}_{V} - \lambda C_{V} - \dot{R}_{V}$	$\dot{R}_{V} = A_{s}J(a,t)$ $R_{V} = e^{-\lambda t} \int_{0}^{t} e^{\lambda x} \dot{R}_{V} dx$ $B_{V} = e^{-\lambda t} \int_{0}^{t} e^{\lambda x} \dot{B}_{V} dx$	$J(\mathbf{a},\mathbf{t}) = \frac{a}{3}\dot{B}\left[\frac{3}{\sqrt{\mu}}\left(\cot h\sqrt{\mu} - \frac{1}{\sqrt{\mu}}\right) - 6e^{-\mu\tau}\sum_{n=1}^{\infty}\frac{e^{-n^{2}\pi^{2}\tau}}{n^{2}\pi^{2}+\mu}\right]$ $H = \dot{R}_{V}/\dot{B}_{V} = \frac{\text{total rate at which atoms are being released}}{\text{total rate at which atoms are being produced}}$ $= \frac{3}{\sqrt{\mu}}\left(\coth\sqrt{\mu} - \frac{1}{\sqrt{\mu}}\right) - 6e^{-\mu\tau}\sum_{n=1}^{\infty}\frac{e^{-n^{2}\pi^{2}\tau}}{n^{2}\pi^{2}+\mu}$ $\approx \begin{cases} \frac{3}{\sqrt{\mu}}erf\sqrt{\mu\tau} - \frac{3}{\mu}\left(1 - e^{-\mu\tau}\right) &, \tau \leq 1/\pi^{2} \\ \frac{3}{\sqrt{\mu}}\left(\coth\sqrt{\mu} - \frac{1}{\sqrt{\mu}}\right) - \frac{6e^{-(\pi^{2}+\mu)\tau}}{\pi^{2}+\mu} &, \tau > 1/\pi^{2} \end{cases}$ $F = R_{V}/B_{V} = \frac{\text{amout of external nondecayed atoms}}{\text{amount of nondecayed atoms in the system}}$ $= \frac{1}{1 - e^{-\mu\tau}} \left[\frac{3}{\sqrt{\mu}}\left(\coth\sqrt{\mu} - \frac{1}{\sqrt{\mu}}\right) - e^{-\mu\tau} + 6\mu e^{-\mu\tau}\sum_{n=1}^{\infty}\frac{e^{-n^{2}\pi^{2}\tau}}{n^{2}\pi^{2}(n^{2}\pi^{2}+\mu)}\right]$	Irradiation phase: $\frac{\partial C}{\partial t} = \dot{B} + \frac{1}{r^{z}} \frac{\partial}{\partial r} \left( r^{z} D \frac{\partial C}{\partial r} \right)$ $C(a, t) = C(r, 0) = 0$ $J(0, t) = 0$ $\frac{dC_{V}}{dt} = \dot{B}_{V} - \dot{R}_{V}$ $B_{V} = C_{V} + R_{V}$	$\dot{R}_{V} = A_{s}J(a,t)$ $R_{V} = \int_{0}^{t} \dot{R}_{V} dx$ $B_{V} = \int_{0}^{t} \dot{B}_{V} dx$	$J(\mathbf{a},\mathbf{t}) = \frac{a}{3}\dot{B}\left(1 - 6\sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2\tau}}{n^2\pi^2}\right)$ $H = \dot{R}_V / \dot{B}_V = \frac{\text{total rate at which atoms are being released}}{\text{total rate at which atoms are being produced}}$ $= 1 - 6\sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2\tau}}{n^2\pi^2} \approx \begin{cases} 6\sqrt{\tau/\pi} - 3\tau &, \tau \le 1/\pi^2 \\ 1 - \frac{6}{\pi^2}e^{-\pi^2\tau} &, \tau > 1/\pi^2 \end{cases}$ $F = R_V / B_V = \frac{\text{amout of atoms released}}{\text{amount of atoms produced in the system}}$ $= 1 - \frac{1}{15\tau} + \frac{6}{\tau} \sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2\tau}}{n^4\pi^4} \approx \begin{cases} 4\sqrt{\frac{\tau}{\pi} - \frac{3}{2}\tau} &, \tau \le 1/\pi^2 \\ 1 - \frac{1}{15\tau} + \frac{6}{\pi^2\tau}e^{-\pi^2\tau} &, \tau > 1/\pi^2 \end{cases}$
$B_{V} = C_{V} + R_{V}$ Heating phase: $\frac{\partial C}{\partial t} = -\lambda C + \frac{1}{r^{z}} \frac{\partial}{\partial r} \left( r^{z} D \frac{\partial C}{\partial r} \right)$ $C(a, t) = 0, C(r, 0) = C^{(0)}$	$\dot{R}_{V} = A_{s}J(a,t)$ $R_{V} = e^{-\lambda t} \int_{a}^{t} e^{\lambda x} \dot{R}_{V} dx$	$= \frac{1}{1 - e^{-\mu\tau}} \begin{bmatrix} \frac{3}{\sqrt{\mu}} \left( erf\sqrt{\mu\tau} - 2\sqrt{\frac{\mu\tau}{\pi}} e^{-\mu\tau} \right) - \frac{3}{\mu} \left[ 1 - (1 + \mu\tau) e^{-\mu\tau} \right] &, \tau \le 1/\pi^2 \\ \frac{3}{\sqrt{\mu}} \left( coth\sqrt{\mu} - \frac{1}{\sqrt{\mu}} \right) - e^{-\mu\tau} + \frac{6\mu e^{-(\pi^2 + \mu)\tau}}{\pi^2(\pi^2 + \mu)} &, \tau > 1/\pi^2 \end{bmatrix}$ $J(\mathbf{a}, \mathbf{t}) = \frac{2C^{(0)}D}{a} \sum_{n=1}^{\infty} e^{-(n^2\pi^2 + \mu)\tau}$ $F^{INT} = R_V / C_V^{(0)} = \frac{\text{amout of external nondecayed atoms}}{\text{amount of atoms at the initial time of heating}}$	Heating phase: $\frac{\partial C}{\partial t} = \frac{1}{r^{z}} \frac{\partial}{\partial r} \left( r^{z} D \frac{\partial C}{\partial r} \right)$ $C(a, t) = 0, C(r, 0) = C^{(0)}$ $J(0, t) = 0$ $\frac{dC_{V}}{dt} = -\dot{R}_{V}$ $0 = C_{V} - C_{V}^{(0)} + R_{V}$	$\dot{R}_{V} = A_{s}J(a,t)$ $R_{V} = \int_{0}^{t} \dot{R}_{V} dx$ $C_{V}^{(0)} = \int_{V} C^{(0)} dV$	$J(\mathbf{a}, \mathbf{t}) = \frac{2C^{(0)}D}{a} \sum_{n=1}^{\infty} e^{-n^2 \pi^2 \tau}$ $F^{INT} = R_V / C_V^{(0)} = \frac{\text{amout of atoms released}}{\text{amount of atoms at the initial time of heating}}$ $= 1 - 6 \sum_{n=1}^{\infty} \frac{e^{-n^2 \pi^2 \tau}}{n^2 \pi^2} \approx \begin{cases} 6\sqrt{\tau/\pi} - 3\tau &, \tau \le 1/\pi^2 \\ 1 - \frac{6}{\pi^2} e^{-\pi^2 \tau} &, \tau > 1/\pi^2 \end{cases}$ $F = \begin{bmatrix} 1 - F_{irr}^{(e)} \end{bmatrix} F^{INT} = \frac{1}{\text{amount of atoms produced in the system until the end of irradiation}}$
$J(0,t) = 0$ $\frac{dC_V}{dt} = -\lambda C_V - \dot{R}_V$	$\int_{C_{0}}^{C_{0}} f(x) = \int_{C_{0}}^{C_{0}} dV$	$= e^{-\mu\tau} \left( 1 - 6\sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2\tau}}{n^2\pi^2} \right) \approx e^{-\mu\tau} \begin{cases} 6\sqrt{\tau/\pi} - 3\tau & , \tau \le 1/\pi^2 \\ 1 - \frac{6}{\pi^2}e^{-\pi^2\tau} & , \tau > 1/\pi^2 \end{cases}$			

## **Calculation Results and Summary**

- The mathematical fractional releases were classified systematically for radioactive and stable isotopes diffusing out of a fuel element under irradiation and accident conditions.
- Only when the diffusing medium is a single layer, it is possible to get an analytical form of fractional release. In other cases, the fractional releases must be calculated numerically.
- The choice of either the fractional release or the fractional release rate depends on whether

#### FR and its rate in a UO<sub>2</sub> kernel during irradiation



FR and its rate in a UO, kernel during heating

the amount generated or the birth rate on which they are based on is more easily identifiable.

According to the fractional releases calculated, the radioactive isotopes <sup>110m</sup>Ag, <sup>137</sup>Cs, <sup>85</sup>Kr and <sup>90</sup>Sr release from a spherical UO<sub>2</sub> kernel more in that order. The strontium release is negligible.



