Muhammet Ayanoglu

NUCE497 - HW5 Solutions

1- There is certain number of oxygen atoms in UO_2 crystal structure depending on the charge state of the U atom. UO_2 stoichiometry represents the ratio of the oxygen to uranium metal and O/M ratio means oxygen to metal ratio. In a perfect UO_2 lattice, this ratio is equal to 2. However, it can vary during the reactor operation which ends up the stoichiometry to go up and down.

Since it is very difficult to measure UO_2 storchiometry, oxygen potential (which can be defined as how likely is the oxygen atom to go after do something else) can be used to determine the stoichiometry.

UO_2 storchiometry is extremely important for the fuel performance since it impacts melting temp, thermal conductivity grain growth, fission gas release, creep, chemical state and behavior of fission products, chemical reactions at inner cladding surface.

Q-2)

a) The grain boundary mobility M_{GB} is given with the following equation:

$$M_{GB} = M_0 \exp\left[-\Theta/k_B T\right] \quad \text{where} \quad \begin{aligned} \Theta &= 2.77 \text{ eV} \\ k_B &= 8.62\times10^{-5} \text{ eV/K} \\ M_0 &= 4.6\times10^{-3} \text{ m}^4/\text{J.s} \end{aligned}$$

Temperature, T, can be calculated by using: $T(r) = T_s + \dfrac{q'}{4\pi k_f}\left[1 - \dfrac{r^2}{R_f^2}\right]$ where $q' = 250$ W/cm, $k_f = 0.028$ W/cm K, $R_f = 0.45$ cm

r [cm]	T [K]	M_{GB} [$\times10^{-18}$ m^4/Js]
@ r = 0	1511	2.65
@ r = $R_f/3$	1432	0.82
@ r = R_f	800	1.7×10^{-8}

b) Average grain size can be obtained by solving following equation numerically:

$$\frac{dD}{dt} = k\left(\frac{1}{D} - \frac{1}{D_m}\right) \quad \text{where} \quad \begin{aligned} k &= 2 M_{GB} V_{GB} \\ D_m &= 2.23\times10^3 \exp\left(-7620/T\right) \end{aligned}$$

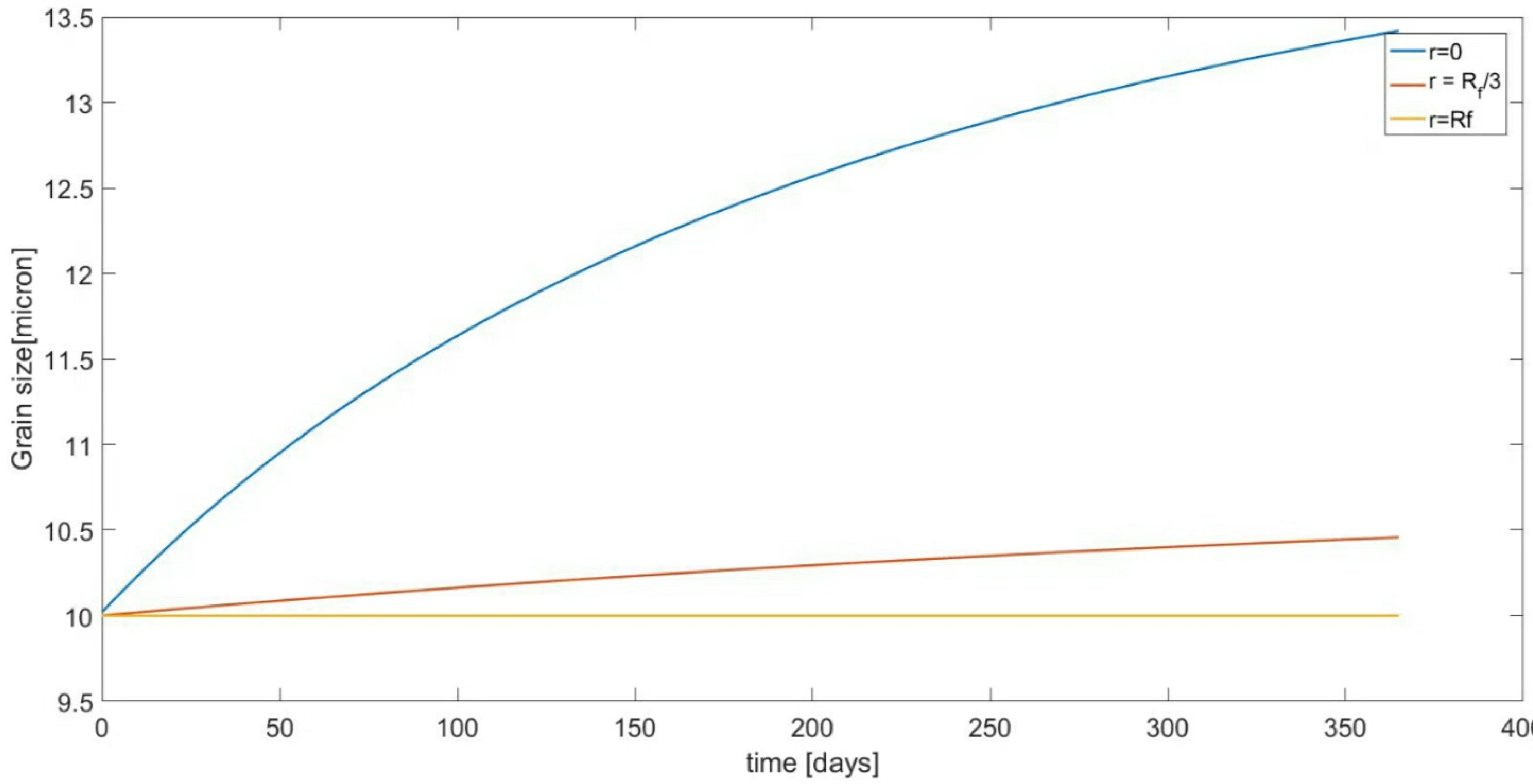
→

$$\frac{dD}{dt} = k\left(\frac{1}{D} + \frac{1}{D_m}\right)$$

$$D[t+dt] = D(t) + dt \cdot k \left[1/D(t) + 1/D_m \right]$$

By using M_{GB} values obtained in part (a); we can calculate the grain size after 1 year:

Distance [cm]	T [K]	M_{GB} [m^4/Js]	k [m^2/s]	D_m [μm]	D [μm] @ t=0	D [μm] @ t=1year
r=0	1511	2.65×10^{-18}	8.38×10^{-18}	14.4	10	13.42
r= Rf/3	1432	0.82×10^{-18}	2.59×10^{-18}	10.9	10	10.46
r= Rf	800	1.66×10^{-26}	5.22×10^{-26}	0.16	10	10



c) Grain size, D, stops evolving with time if $\frac{dD}{dt}=0$ which yields $D=D_m$. Based on the results obtained in part b, this is satisfied at $r=R_f$. On the other hand, it takes more than 3 years for the grains at r=0 and r=Rf/3 to stop evolving with time.

Q-3) a) $PV = n_{He} RT$ where $P = 2$ MPa

$T = 273K$

$R = 8.314$ MPa-cm^3/mol-K

$V = V_{gap} + V_{plenum} = \pi \left[R_{ci}^2 - R_f^2 \right] h_{pellet} + \pi R_{ci}^2 h_{plenum}$

$= \pi . (10 \times 0.119)(0.418^2 - 0.41^2) + \pi (0.418^2)(0.6)$

$= 0.577$ cm^3

$$n_{He} = \frac{(2)(0.577)}{(8.314)(273)}$$

$$\boxed{n_{He} = 5.1 \times 10^{-4} \text{ moles}}$$

b) Temperature change cross the fuel pellet is given as $\Delta T(r) = \frac{LHR}{4\pi k_f} \left[1 - \frac{r^2}{R_f^2} \right]$.

The average temperature can then be written as:

$$\overline{\Delta T} = \frac{1}{\pi R_f^2} \int_0^{R_f} \Delta T(r) \, 2\pi r \, dr$$

$$= \frac{1}{\pi R_f^2} \int_0^{R_f} \left[A + Br^2 \right] 2\pi r \, dr \quad \text{where} \quad A = \frac{LHR}{4\pi k_f}$$

$$B = -\frac{LHR}{4\pi k_f R_f^2}$$

$$= \frac{1}{\pi R_f^2} \left(\frac{2\pi r^2}{2} A + \frac{2\pi r^4}{4} B \right)_0^{R_f}$$

$$= \frac{1}{\pi R_f^2} \left[\pi R_f^2 A + \frac{\pi R_f^4 B}{2} \right]$$

$$\overline{\Delta T} = A + \frac{B R_f^2}{2}$$

$$= \frac{LHR}{4\pi k_f} - \frac{LHR}{4\pi k_f R_f^2} \left(\frac{R_f^2}{2} \right)$$

$$= \frac{LHR}{4\pi k_f} \left(1 - \frac{1}{2} \right)$$

$$\overline{\Delta T} = \frac{LHR}{8\pi k_f}$$

$\longrightarrow$

$$\Delta T = \frac{LHR}{8\pi k_f}$$

$k_f = 0.03 \; W/cm\,K$

$$LHR = \frac{Q}{\pi R_f^2} = 246 \; W/cm \rightarrow \text{calculated for } \phi = 2.75\times10^{13} \; n/cm^2 s, \; q = 4.2 \; wt\%$$

$$\Delta T = \frac{246}{8\pi(0.03)} = 326 \; K$$

c) Since $\phi \rightarrow \phi(t)$, then $\dot{F} \rightarrow \dot{F}(t)$ and therefore $N_{FG} = y\dot{F}t \rightarrow N_{FG} = y\int_0^{2yr} \dot{F}(t)\,dt$

$$N_{FG} = y\int_0^{t_1} \dot{F}(t)\,dt$$

$$= y\left[\int_0^{t_r} \dot{F}_1(t)\,dt + \int_{t_r}^{t_1} \dot{F}_2(t)\,dt\right]$$

where

$\dot{F}_1(t) = q N_u \sigma_f \phi_0 \frac{t}{3\times3600}$

$\dot{F}_2(t) = q N_u \sigma_f \phi_0$

$t_r = 3\times3600 \; s$

$t_1 = 2\times365\times24\times3600 \; s$

$$= y\left[\int_0^{t_r} q N_u \sigma_f \phi_0 \frac{t}{t_r}\,dt + \int_{t_r}^{t_1} q N_u \sigma_f \phi_0\,dt\right]$$

$$= y\left[q N_u \sigma_f \phi_0 \frac{t^2}{2t_r}\Big|_0^{t_r} + q N_u \sigma_f \phi_0 t\Big|_{t_r}^{t_1}\right]$$

$$= y\left[q N_u \sigma_f \phi_0 \frac{t_r}{2} + q N_u \sigma_f \phi_0 (t_1 - t_r)\right]$$

$$= y\, q N_u \sigma_f \phi_0 \left(t_1 - \frac{t_r}{2}\right)$$

$$= (0.3)(0.042)(2.44\times10^{22})(550\times10^{-24})(2.75\times10^{13})\left(2\times365\times24\times3600 - \frac{2\times3600}{2}\right)$$

$N_{FG} = 2.93\times10^{20}$ fission gas atoms/cm³

$\longrightarrow$

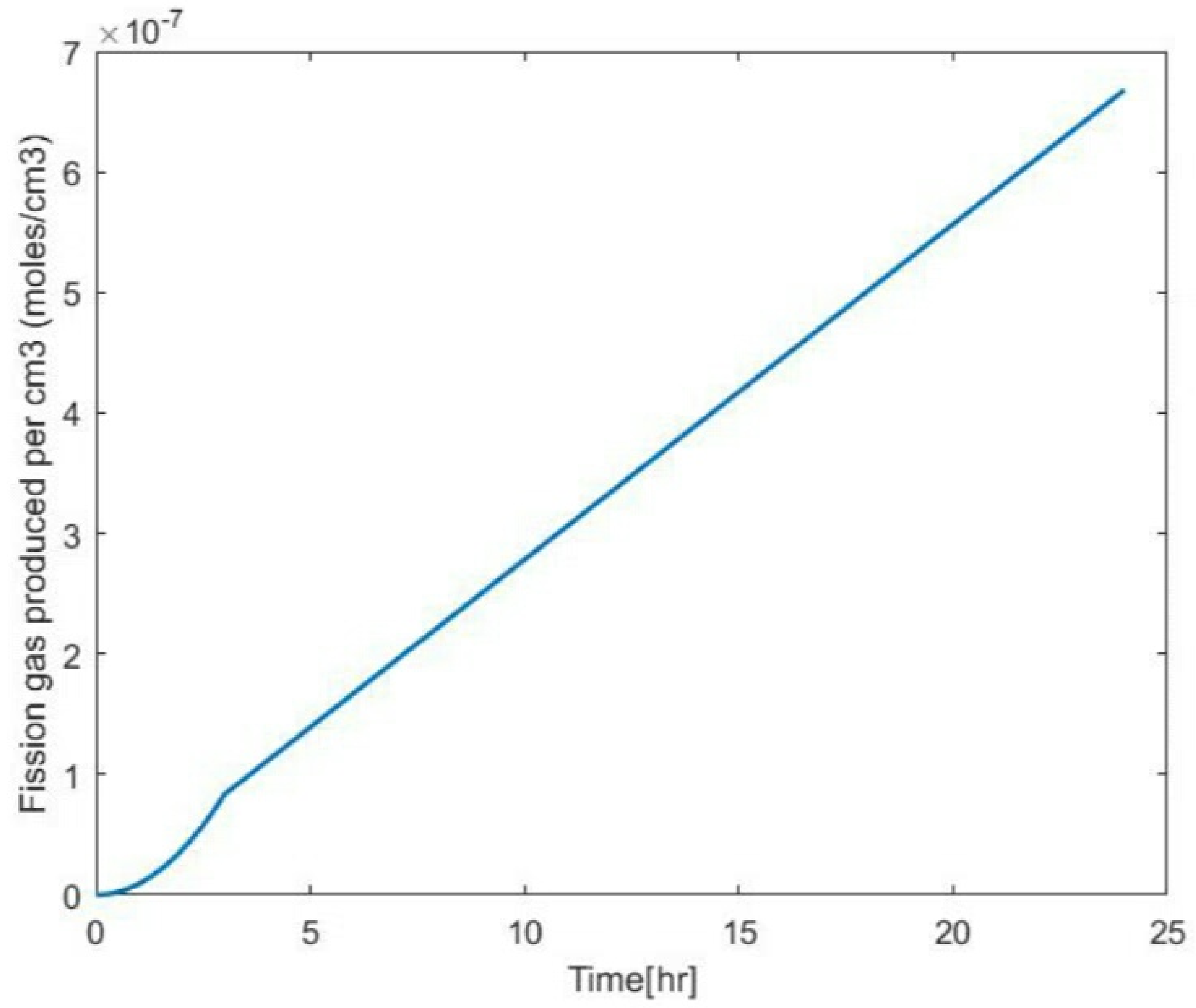
$N_{gas} = N_{FG} \cdot \text{Volume}$

$= (2.93\times10^{20})(0.577\ cm^3)$

$N_{gas} = 1.69 \times 10^{20}$ fission gas atoms

OR

$= 2.81\times10^{-4}$ moles



d)

The amount of fission gas released to the gap can be calculated if fraction of fission gas released, f, is known. It can be obtained by using following equations:

$$f = 4\sqrt{\frac{D \cdot t}{\pi a^2}} - \frac{3}{2}\frac{D t}{a^2} \quad \text{where} \quad D = D_1 + D_2 + D_3$$

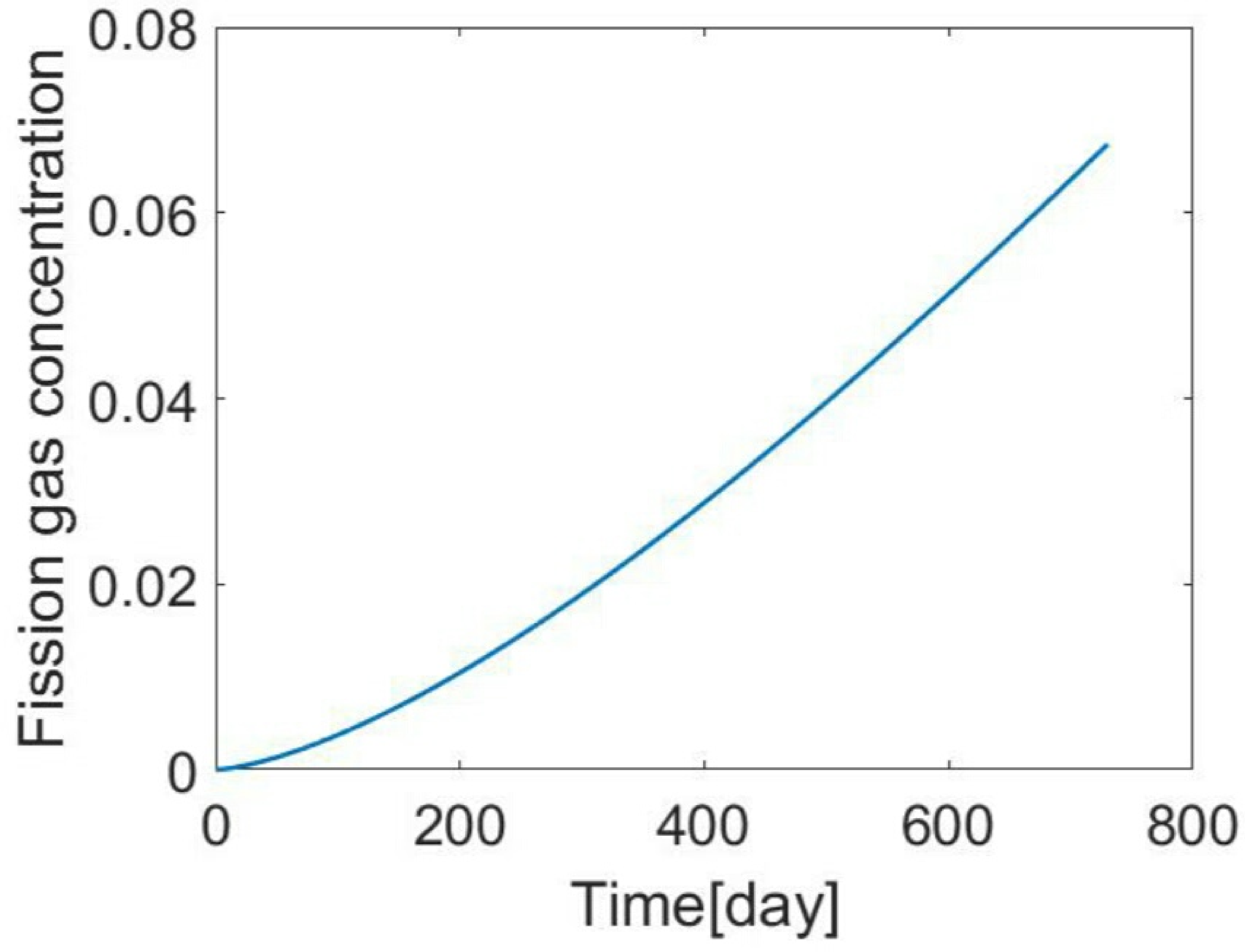
$\rightarrow 2\times10^{-36}\ \dot{F}$

$\rightarrow 1.41\times10^{-21}\ \exp\left(\frac{-1.19}{k_B T}\right) \cdot \sqrt{\dot{F}}$ and $T \rightarrow \bar{T}$, $\dot{F} \rightarrow \dot{F}(t)$

$\rightarrow 7.6\times10^{-6}\ \exp\left(-\frac{3.03}{k_B T}\right)$

Concentration of fission gas in the gap and plenum then can be calculated as:

$$C = \frac{f \cdot N_{gas}}{N_{gas} + N_{He}}$$



e) This equations can be simply added inside of a MATLAB function similar to what was done in the homework. Every time step, the amount fission gas released to the gap will be calculated. By using new concentration value, gap conductivity will be calculated.

Q-4) a) Total volumetric change in a fuel pellet through the time is calculated as:

$$\varepsilon_{total} = \underbrace{\boxed{\varepsilon_{th}}}_{\text{thermal expansion}} + \underbrace{\boxed{\varepsilon_{D}}}_{\text{densification}} + \overbrace{\boxed{\varepsilon_{SFP}}}^{\text{solid swelling}} + \underbrace{\boxed{\varepsilon_{GFP}}}_{\text{Gaseous swelling}}$$

Now, we will calculate volumetric change due to each mechanism:

Thermal expansion:

$$\varepsilon_{th} = \alpha\left[\bar{T} - T_{fab}\right] \quad \text{where} \quad \alpha = 11\times10^{-6}\ {}^{1}/_{K}$$

$$\bar{T} = 1126\ K$$

$$T_{fab} = 300\ K$$

$$= 11\times10^{-6}\left[1126 - 300\right]$$

$$\boxed{\varepsilon_{th} = 9.1\times10^{-3}}$$

Densification:

$$\varepsilon_D = \Delta\rho_0\left[\exp\left(\frac{\beta \ln 0.01}{C_D\,\beta_D}\right) - 1\right] \quad \text{where}$$

$C_D = 1$, because we are higher than $750^\circ C$

$\beta_d = 5/950 = 0.0053$ FIMA

$\Delta\rho_0 = 0.01$

$$\beta = \frac{\int_0^t \dot{F}(t)\,dt}{N_u} \quad \text{where} \quad \int_0^t \dot{F}(t)\,dt = q\,\sigma_f N_u \phi_0\left[t_1 - \frac{t_R}{2}\right]$$ from previous question

$$\beta = q\,\sigma_f\,\phi_0\left[t_1 - \frac{t_R}{2}\right]$$

$$= (0.042)(550\times10^{-24})(2.75\times10^{13})\left[2\times365\times24\times3600 - \frac{2\times3600}{2}\right]$$

$$\beta = 0.04 \text{ FIMA}$$

$$= 0.01\left[\exp\left(\frac{0.04 \ln 0.01}{1\ \ 0.0053}\right) - 1\right]$$

$$\boxed{\varepsilon_D \cong -0.01}$$

Solid fission product swelling:

$$\varepsilon_{SFP} = 5.577\times10^{-2}\,\rho\,\beta \quad \text{where} \quad \rho = \text{initial } UO_2 \text{ density} = 10.97$$

$$= 5.577\times10^{-2}(10.97)(0.04) \qquad \beta = 0.04 \text{ FIMA}$$

$$\boxed{\varepsilon_{SFP} = 0.025}$$

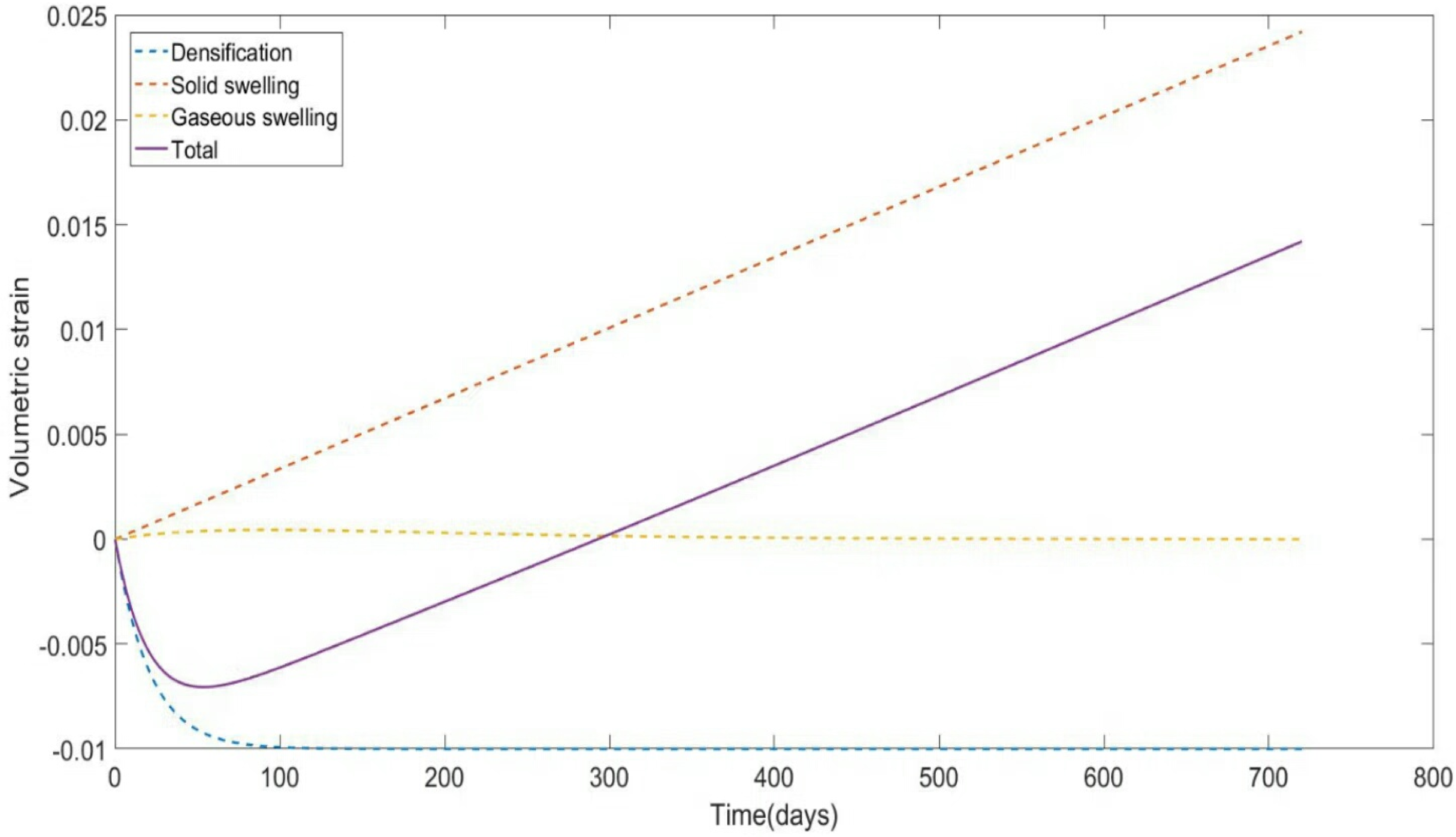
Gaseous fission product swelling:

$$\varepsilon_{GFP} = 1.96\times10^{-28}\,\rho\,\beta\,(2800 - T)^{11.73}\,e^{-0.0162(2800-T)}\,e^{-17.8\rho\beta}$$

$$= 1.96\times10^{-28}(10.97)(0.04)(2800 - 1126)^{11.73}\,e^{-0.0162(2800-1126)}\,e^{-17.8(10.97)(0.04)}$$

$$\boxed{\varepsilon_{GFP} = 3.8\times10^{-6}}$$

$$\varepsilon_{tot} = 9.1\times10^{-3} - 0.01 + 0.025 + 3.8\times10^{-6} = 0.024$$



b) In this part, we will follow the same procedure as HW3-Q1. However, we will not only have thermal expansion but also contribution from densification, solid/gaseous fission products as well.

while

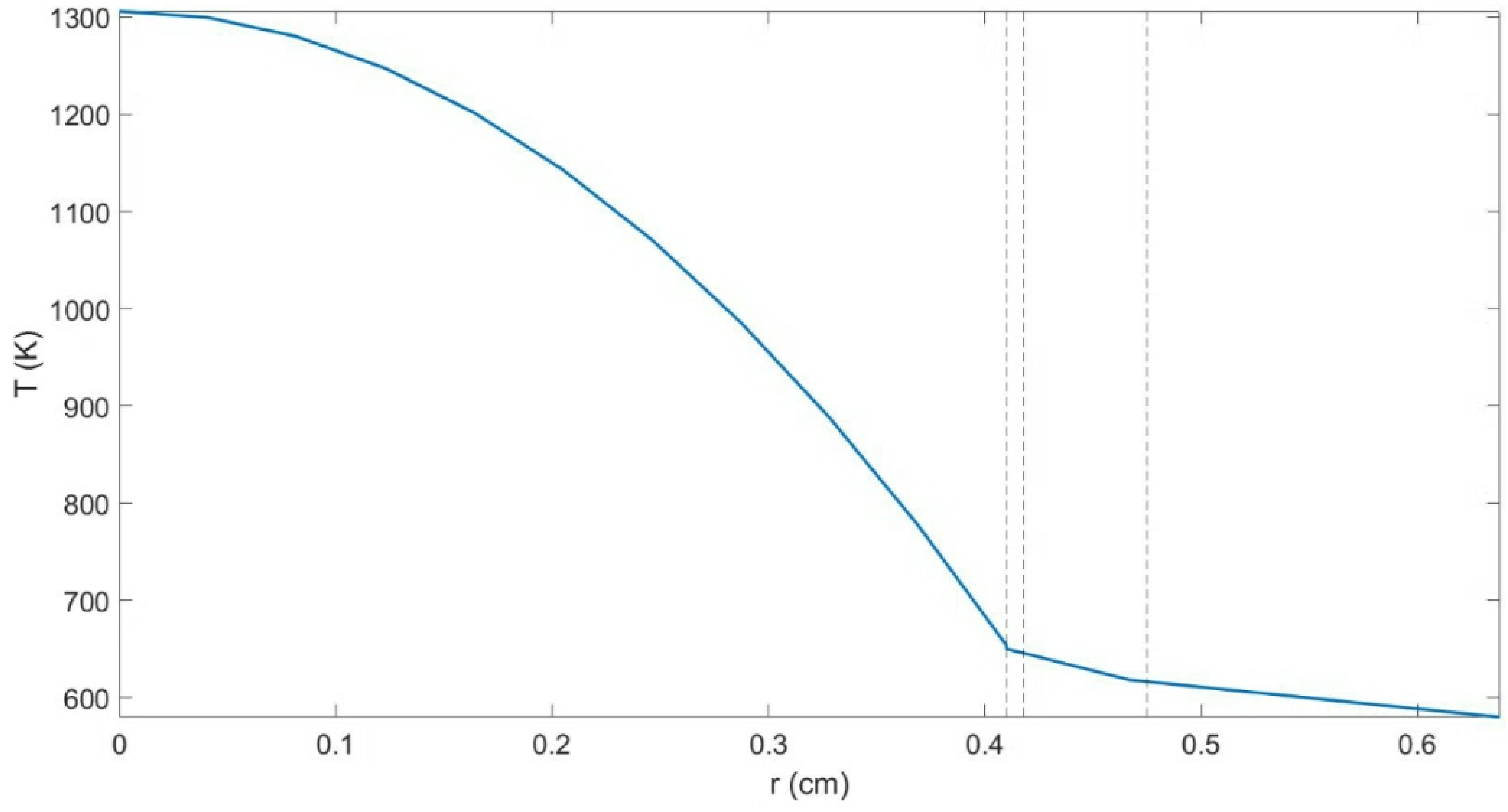
$\varepsilon_{th} = \dots$
$\varepsilon_{D} = \dots$
$\varepsilon_{SFP} = \dots$
$\varepsilon_{GFP} = \dots$

these values are calculated for the end of life of the fuel rodlet.

$\varepsilon_{tot} = \varepsilon_{th} + \varepsilon_D + \varepsilon_{SFP} + \varepsilon_{GFP}$
$Ch\_fuel = \varepsilon_{tot} * R_f$

< SAME AS HW3_Q1 >

end



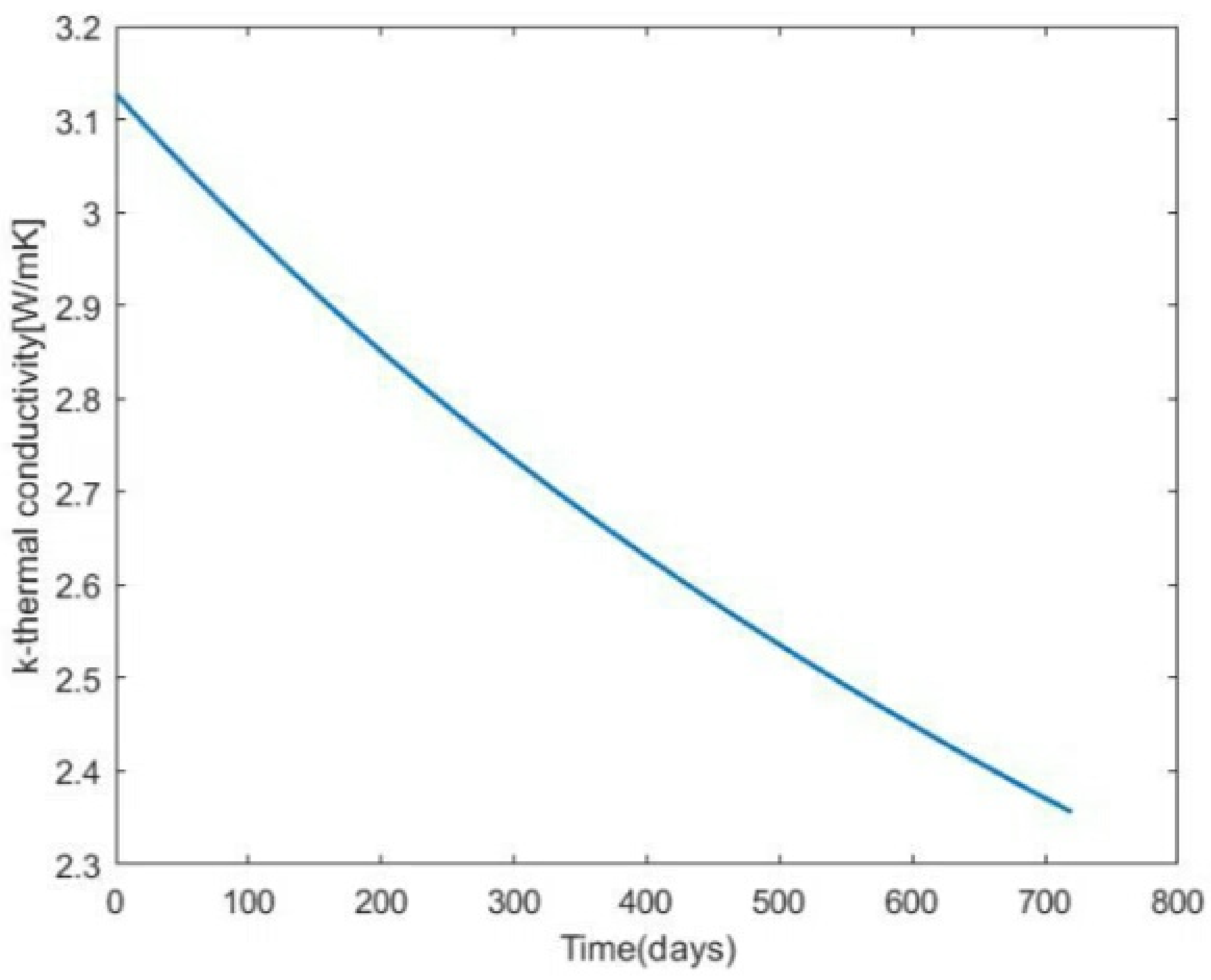
c) This equations can be simply added inside of a MATLAB function similar to what was done in the homework. Every time step, the amount volumetric change in fuel will be calculated. By using this information, gap size (and conductance) will be calculated iteratively.

Q-5)

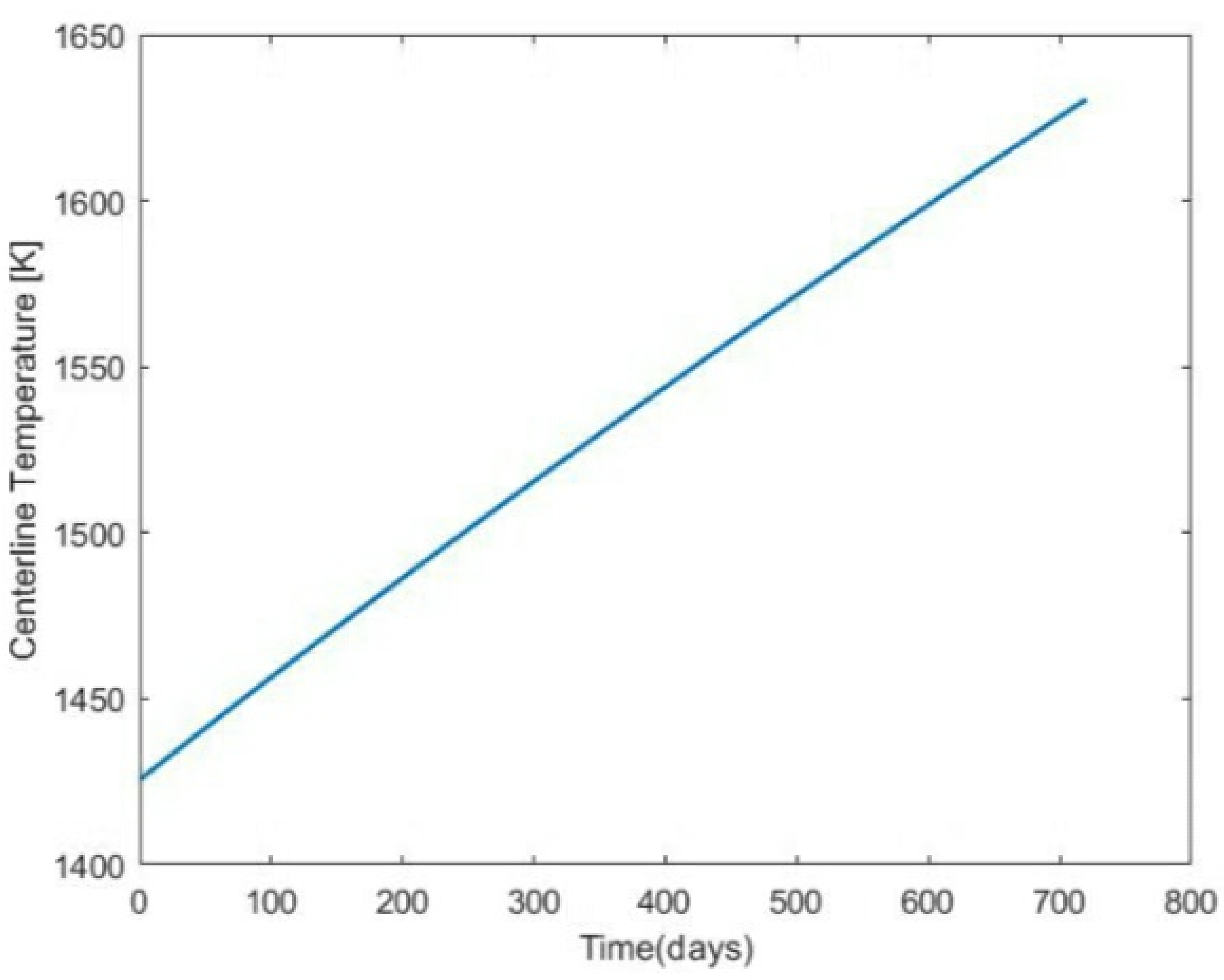
$$k = (1 - R_f(T))k_{ph1}(T,\beta) + R_f(T)k_{ph2}(T,\beta) + k_{el}(T)$$
$$R_f(T) = \frac{1}{2}\left(1 + \tanh\left(\frac{T-900}{150}\right)\right)$$
$$k_{ph1} = \frac{1}{(9.592\times10^{-2} + 6.14\times10^{-3}\beta - 1.4\times10^{-5}\beta^2 + (2.5\times10^{-4} - 1.81\times10^{-6}\beta)T}$$
$$k_{ph2} = \frac{1}{(9.592\times10^{-2} + 2.6\times10^{-3}\cdot\beta + (2.5\times10^{-4} - 2.7\times10^{-7}\beta)T}$$
$$k_{el} = 1.32\times10^{-2}e^{1.88\times10^{-3}T}$$

Note that $T \rightarrow$ °C
$\beta \rightarrow$ MWd/kgU

a)



b) $T_0 = T_s + \frac{LHR}{4\pi k}$



c) This equations can be simply added inside of a MATLAB function similar to what was done in the homework. Every time step, the fuel thermal conductivity will be calculated as a function of burnup. Then, the temperature @ new time step will be calculated by using new k.