# Modelling of High Burnup Fuel Pulverization Behavior by FRAPCON4.0 / FRAPTRAN 2.0

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#### 1. Introduction

The phenomenon of fuel pulverization is caused by the overpressure of grain boundary bubbles in both the normal and high burn-up structures under rapid heating conditions. The rapid increase of temperature and drop in hydrostatic pressure surrounding fuel pellets make over-pressurization of the intergranular bubbles, which tears grain boundary cracks to pulverize the fuel. The pulverized fuel flows down into the gap between the fuel and the cladding and causes local heating. This leads to further severe deformation of the cladding and fuel dispersal to the primary system. Threshold pressure in the intergranular pore for tearing grain boundary has been proposed in many studies. [1-5] Threshold pressure considers not only fission gas pressure, but bubble capillary pressure of bubble and hydrostatic pressure in the surrounding pellet. Additionally, to take into account that tearing becomes easier when the bubbles are closely located to each other, another criteria also consider the bubble coverage fraction on grain face. In this study, the size and number density information of intergranular fission gas bubbles during the normal operation conditions of light water reactors were derived using a modified FRAPCON 4.0 code. Based on the calculated intergranular bubble size, modified FRAPTRAN 2.0 was used to determine pellet pulverization in the situation of loss of coolant accident (LOCA) or reactivity initiated accident (RIA).

# 2. Methodology for calculating grain boundary bubble size and pulverization modelling

The calculation was performed in different ways by dividing the pellet into a high burnup structure formed in the rim part of the pellet and a normal structure in the center part. The gas pressure inside the fission gas is so high and the gas atom density is also high that the attraction between fission gas atoms cannot be neglected, so the ideal gas equation as an equation of state cannot be used. The equation of state of gas in the fission gas bubble was used by Xiao et al. [6]

$$P = \frac{RT}{V} \left( 1 + \frac{c}{V - b} \right) - \frac{a}{V^2} \tag{1}$$

P = pressure [Pa] V = volume/mole [m<sup>3</sup>/mol]T = temperature [K] R = gas constant [J/mol K]a = 0.25978 [J m<sup>3</sup>/mol<sup>2</sup>]b = 2.39276 × 10<sup>-5</sup> [m<sup>3</sup>/mol]c = 5.56583 × 10<sup>-5</sup> [m<sup>3</sup>/mol]

#### 4.1 Calculation in normal structure region

The pressure in the grain boundary bubbles was assumed to be the sum of the bubble capillary pressure and hydrostatic pressure calculated by FRAPCON 4.0. The area density of grain boundary bubble and radius in the normal structure of centerline has the following relationship

$$n_b[^{\#}/_{m^2}] = \frac{3.0 \times 10^{13}}{1 + 6.0 \times 10^{13} (\pi r_b^2 - 2.83 \times 10^{-15})} \tag{2}$$

Assuming that the dihedral angle of  $UO_2$  is 50 degrees, the volume of the lenticular bubble according to the bubble radius is as follows.

$$\frac{4\pi r^3}{3} \frac{2 - 3\cos 50 + \cos^3 50}{2\sin^3 50} \tag{3}$$

Using equations  $(1) \sim (3)$  and temperature, the amount of grain boundary fission gas, pressure of bubbles calculated in FRAPCON 4.0, the intergranular bubble radius in each time step, axial node, and radial node of the simulation can be calculated.

#### 4.2 Calculation in high burnup structure region

If the pellet average burnup exceeds about 50 GWd/tU, a unique microstructure called high burnup structure is formed. This special microstructure has a porosity of 20% or more and a spherical bubble shape, not a lenticular shape. The method is similar to the normal structure, but the bubble number density follows the equation below.

$$n_p[\#/m^2] = 4.5 \times 10^{14} \times \exp\left\{(0.038846)(Bu - 0.2Bu_{av})\right\}$$
(4)

The above equation is another empirical formula for pore density in a high burnup structure. [7] Ronchi et al. proposed the pore pressure as follows in consideration of the over-pressurization of gas bubbles in the high burnup structure and suggested that a proper C value as 55 N/m [8]

$$P = \frac{2\gamma}{r} + \frac{Gb}{r} = \frac{C}{r} \tag{5}$$

Similarly, if Xiao's equation of state is applied, then the radius of the bubble can be calculated with FRAPCON 4.0 data and equation (1), (5).

### 4.2 Pulverization modelling

For pulverization modeling, a threshold pressure for pulverization was used. The critical pressure of Chakraborty et al[4] below was used.

$$P^{cr} = P_h + P_s + \frac{1}{F_4} \sqrt{\frac{\pi E g_{gb}}{(1 - v^2)r}}$$

$$F_4 = \pi (0.568\varphi^2 + 0.059\varphi + 0.5587) + \frac{1}{F_4}$$

$$F_h = \text{Hydrostatic pressure [Pa]}$$
(6)

- $P_h = \text{Capillary pressure [Pa]}$
- $P_h$  = Young's modulus of UO<sub>2</sub> [Pa] .
- $P_h = \text{Grain boundary fracture energy of UO}_2 [J/m^2]$
- $P_h =$  Poisson's ratio
- $P_h$  = Bubble coverage fraction on grain face -

In the hydrostatic pressure, pellet cladding mechanical interaction, cladding ballooning and burst were also considered. In LOCA or RIA simulation in FRAPTRAN 2.0, the temperature of each radial node of fuel rod was calculated at each time step, and pulverization was assumed to occur in the radial node when the pressure inside the pores exceeded the critical pressure due to the temperature increase.

# 3. Calculate bubble size and bubble pressure

Figure.1 shows the radial intergranular pore size and pressure distribution of 91.35 GWd/tU UO2 nuclear fuel calculated using the modified FRAPCON4.0 by adding the above methodology to the code. In the core of the nuclear fuel, the intergranular bubbles are agglomerated to create a tunnel so that bubble growth no longer occurs, so the size and bubble pressure are kept constant. It can be seen that the shape of the graph changes rapidly in the area where the high burnup structure is formed outside the nuclear fuel. From the normal structure in the center toward the high burnup structure of the rim part, the bubble size decreases and then increases significantly when entering the high burnup structure area while the bubble pressure increases as it goes radially outward and stops increasing when entering the high burnup structure area. Overall, the pressure of the bubbles in the high burnup structure is higher than that of the bubbles in the normal structure during the normal operation of reactors, which

can explain the reason why pulverization occurs more easily at the outside part than the nuclear fuel center in LOCA or RIA situations. When the temperature of the fuel rises in a transient condition, the intergranular bubbles in the outside of the fuel, which have higher pressure during the normal operation, more easily reach the critical pressure.



Figure. 1 Calculated intergranular bubble radius and pressure of 91.35 GWd/tU UO<sub>2</sub>

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