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Crack Stability in Breached Fuel

Spent Fuel and Waste Disposition

Prepared for
U.S. Department of Energy
Spent Fuel and Waste Science and Technology

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EXECUTIVE SUMMARY

This report describes the fracture mechanics formalism to evaluate the stability of cracks in a fuel cladding. Recognized consensus-body linear elastic fracture mechanics (LEFM) was applied to identify the crack instability length, or the length at which unstable mechanical crack extension would occur, as a function of pellet swelling loading (radial strain and fraction conversion from UO_2 to U_3O_8) at the local cracked cladding region for two postulated fracture toughness (K_{IC}) values of the cladding. The crack opening displacement (COD) and the crack opening area (COA) were also identified. This analysis informs evaluations for crack extension and the potential for pellet debris loss from the fuel rod for cases of pellet oxidation in dry storage canisters where inadvertent residual water may undergo radiolysis causing oxidizing conditions to pellets exposed to the canister environment through breached cladding.

The Timoshenko solution [8] was first used to estimate the press-set pressure exerted by the oxidized pellet on the cladding. Based on the pressure, the stress in the cladding was obtained from the classic solution of a pressurized cylindrical structure; and the strain was calculated from linear elasticity (Hooke's law). In the present analysis, initial contact between the cladding and the pellet (no gaps) is assumed to have taken place from reactor operation.[1] This approach inevitable leads to a very high stress state far exceeding the elastic limit of the cladding material. Therefore, the subsequent LEFM analysis results in a conservative (short) critical crack length with a corresponding critical crack opening area/displacement. For example, in the early stage of oxidized pellet-cladding interaction (OPCI), when only 10% of UO_2 is converted to U_3O_8, the critical crack length is estimated as 0.15 mm for K_{IC} = 25 MPa$\sqrt{m}$ and is 1.32 mm for K_{IC} =90 MPa$\sqrt{m}$, and the corresponding crack opening displacements are 5 μm and 52 μm, respectively. This small crack opening would preclude large pellet debris from leaving the rod.

It is expected that the extent of growth from an unstable crack to a stable crack is limited by the extent of additional pellet oxidation and swelling along the length of the rod from the crack site. In other words, continued crack extension beyond only a local region of pellet oxidization would not occur due to removal of the displacement-based loading condition although the demonstration thereof was not possible with the present two-dimensional model in this analysis.[2]

Additional improvements for evaluation of flaw tolerance under pellet swelling loading are suggested. Additional characterization of the fracture toughness of High-Burnup (HBU) cladding is also suggested.

This report fulfills the M4 milestone M4SF-21SR010203045, "Crack Opening in Breached Fuel" under Work Package Number SF-21SR01020304.

[1] The design initial pellet/clad gap of 0.107 mm is assumed to be closed through fuel burnup and pellet expansion therewith. The details for evaluation of pellet swelling with oxidation are provided in Appendix A to this present report.

[2] Above the critical crack length (crack instability length) determined by the fracture toughness K_{IC}, crack propagation would occur unless there is crack arrest. Crack arrest would occur if crack loading conditions result in a fall of the applied stress intensity to K_{Ia}, the crack-arrest fracture toughness of the cladding.

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ACRONYMS

B&W	Babcock & Wilcox
COA	Crack opening area
COD	Crack opening displacement
DOE	U.S. Department of Energy
HBU	High Burn-Up
ID	Inner diameter
LEFM	Linear Elastic Fracture Mechanics
LWR	Light Water Reactor
NE	Nuclear Energy
NEUP	Nuclear Energy University Program
NRC	Nuclear Regulatory Commission
OD	Outer diameter
OPCI	Oxidized Pellet-Cladding Interaction
PWR	Pressurized Water Reactor
PNNL	Pacific Northwest National Laboratory
RH	Relative Humidity
SFWD	Spent Fuel and Waste Disposition
SINTAP	Structural INTegrity Assessment Procedures
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
SNTT	Spiral Notch Torsion Test
SRNL	Savannah River National Laboratory
TD	Theoretical Density

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1. INTRODUCTION

The experiments conducted by Einziger and Cook (1985) [1], Einziger and Strain (1986) [2], and Novak and Hastings (1984) [3] have demonstrated that pellet oxidation caused by small cladding defects could breach the fuel rod under dry storage of the spent nuclear fuel (SNF). In the process of pellet oxidation, the uranium dioxide (UO_2) may convert to triuranium octoxide (U_3O_8). As the uranium oxide experiences this transformation, its density changes from 10.96 g/cm^3 to 8.35 g/cm^3, which leads to pellet volume expansion, and these affected pellets would have already been in contact with cladding inner diameter. The oxidizing pellets may continue to swell and could eventually exert sufficient stress on the cladding to initiate crack propagation from the original defect. This action could split the fuel rod axially.

This report focuses on the evaluation of the cladding stress and fracture due to pellet volume and diametrical changes as UO_2 converts to U_3O_8 by oxidation. The kinetics of uranium oxide transformation and the burnup dependence [4], the fracture of pellets [5], and the rim formed on pellet surface when the local burnup exceeds about 40 GWd/MTU [6, 7] are not considered here, but the initial condition of direct contact between the fuel pellet and cladding is taken into consideration. That is, the fuel-clad gap is set to be closed as UO_2 begins to convert to U_3O_8 in the present analysis.

Timoshenko solutions [11] are used to estimate the press-fit pressure exerted by the pellet due to volume/diametrical increase against the cladding. For generality, thick-wall cylinder solutions and Hooke's law are used to calculate the stresses and strains on the cladding based on the press-fit pressure. The details can be found in Section 2. It follows in Section 3 that the cladding hoop stress is input to API 579-1/ASME FFS-1 Fitness-For-Service code [12] for calculating stress intensity factor (K) for a length $2c$ of through-wall crack in a fuel rod cladding. The critical crack length and critical crack opening area (COA) can be obtained by comparing the calculated K to the cladding fracture toughness K_{IC}. Two values of K_{IC} (25 and 90 MPa$\sqrt{\text{m}}$) are selected in the calculation to cover the possible range of the material property. The crack length corresponding to the condition $K = K_{IC}$ is defined as the critical crack length, from which the critical crack opening area and the critical crack opening displacement can be calculated. Lastly, the results and path forward are discussed in Section 4. Appendix A details the derivation of equations used to estimate pellet volume increase due to oxidation, and Appendix B is provided for alternative methods to calculate K and COA. It can be seen that the API 579 procedure would provide the most conservative results.

The extent of crack extension from an unstable crack at the critical crack length to a stable crack, and similarly the extent of crack opening area, and crack opening displacement are limited by the extent of additional pellet oxidation along the length of the rod. In other words, crack extension beyond a local region of pellet oxidization would not occur due to removal of the applied displacement-based loading condition. The extent of pellet oxidation up the fuel rod is beyond the scope of this report. No evaluation is attempted for loss of pellet fragments from an opened crack, or for the relief on cladding press-fit pressure due to loss of pellet fragments.

2. STRESS ANALYSIS OF OXIDIZED PELLET-CLADDING INTERACTION (OPCI)

This section describes a linear elastic approach to calculate cladding failure stress and deformation as a result of the oxidized pellet-cladding interaction (OPCI), and to estimate the critical crack length, crack opening area, and opening displacement based on the principle of Linear Elastic Fracture Mechanics (LEFM) and a set of bounding cladding fracture toughness (K_{IC}), which is considered as a material property.

The Babcock & Wilcox (B&W) 15 x 15 pressurized water reactor (PWR) fuel assembly with 208 fuel rods [8] is chosen as a representative system for the current analysis. The fuel as-designed parameters are list below [9, 10]:

- Fuel rod outer diameter (OD) or cladding OD: 10.922 mm (0.430 in.)
- Cladding inner diameter (ID): 9.576 mm (0.377 in.)
- Cladding Thickness 0.673 mm (0.0265 in.)
- Cladding material: Zircaloy-4 (Zr-4)
- Pellet diameter: 9.362 mm (0.3686 in.)
- Pellet Length: 15.24 mm (0.600 in.)
- As-designed diametrical gap (Cladding ID minus pellet diameter): 214 μm (0.214 mm or 8.4 mil); Radially, it is 0.214/2= 0.107 mm between the pellet and the cladding.

Additional pellet information [9]:

- Fuel pellet density: 95% Theoretical Density (TD)
- TD of stoichiometric UO_2: 10.96 g/cm^3

2.1 General Solution for a Pressurized Cylinder

The cladding is a relatively thin shell structure with R_i/t = 7.11, where R_i is the inner radius of the fuel rod (or cladding) and t is the cladding wall thickness). For generality purposes, the stress solution for thick-wall cylinder is presented below and will be used throughout this report.

For a cylinder with outside radius R_o and inner radius R_i subjected to internal pressure p_i and external pressure p_o, Timoshenko [11] showed that

$$\sigma_h = \frac{p_i R_i^2 - p_o R_o^2 + (p_i - p_o) R_i^2 R_o^2 / r^2}{R_o^2 - R_i^2} \tag{1}$$

$$\sigma_r = \frac{p_i R_i^2 - p_o R_o^2 - (p_i - p_o) R_i^2 R_o^2 / r^2}{R_o^2 - R_i^2} \tag{2}$$

where σ_h is the circumferential or hoop stress at a radial distance r from the center of the cylinder, σ_r is the radial stress, and the axial stress is not considered in the present case. As expected, Eq. 2 suggests that $\sigma_r = 0$ on unpressurized surface of the cylinder and $\sigma_r = -p$ on pressurized surface.

2.2 Press fit Solution for Oxidized Pellet-Cladding Interaction (OPCI)

Figure 1 shows that two hollow cylinders are press-fitted against each other at $r = R$ with a radial interference δ_R. The outer cylinder has material properties Young's modulus (E_o) and Poisson's ratio (v_o). For the inner cylinder, these material properties are denoted as E_i and v_i.

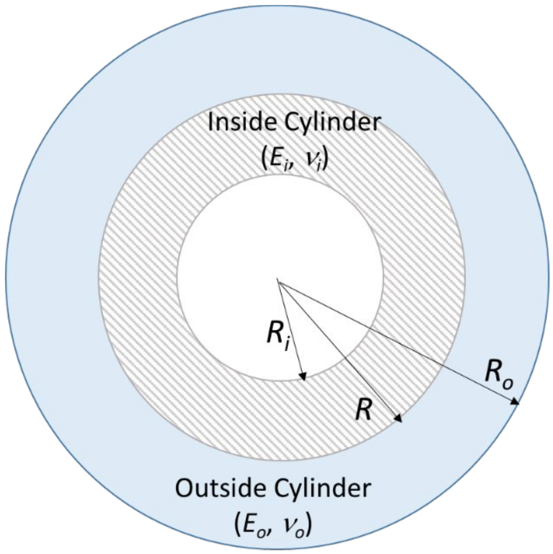


Figure 1. Press fit of two cylinders

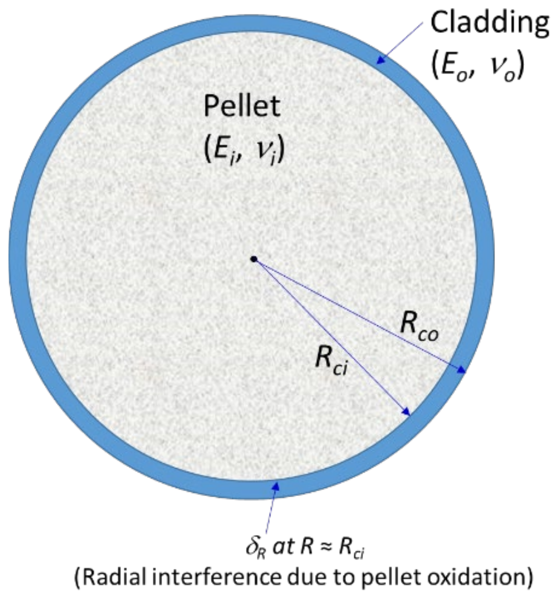


Figure 2. Oxidizing pellet stresses the cladding (not to scale)

2.2.1 Cladding Stresses

The interface pressure (press-fit or shrink-fit pressure), p, can be expressed as [11]

$$p = \frac{\delta_R}{\frac{R}{E_o}\left(\frac{R_o^2+R^2}{R_o^2-R^2}+\nu_o\right)+\frac{R}{E_i}\left(\frac{R^2+R_i^2}{R^2-R_i^2}-\nu_i\right)} \tag{3}$$

In the case of OPCI (see Fig. 2), the following parameters are used in Eq. 3: $R = R_{ci}$, which is the cladding inner radius; $R_o = R_{co}$, which is the cladding or fuel rod outer radius; $R_i = 0$ (solid pellet); δ_R is the radial growth of the pellet due to oxidation, E_o is the Young's modulus of the cladding, ν_o is the Poisson's ratio of the cladding, E_i is the Young's modulus of the pellet, and ν_i is the Poisson's ratio of the pellet. The resulting expressions for the cladding stresses are

Hoop (or circumferential) stress at the cladding inner diameter: $\sigma_{ch} = p\frac{R_{co}^2+R_{ci}^2}{R_{co}^2-R_{ci}^2}$ (4)

Radial stress at the cladding inner diameter: $\sigma_{cr} = -p$ (5)

Hoop stress at the cladding outer diameter: $\sigma_{oh} = 2p\frac{R_{ci}^2}{R_{co}^2-R_{ci}^2}$ (6)

Radial stress at the cladding outer diameter: $\sigma_{or} = 0$ (7)

Note that σ_{ch} (Eq. 4) is always greater than σ_{oh} (Eq. 6). For conservatism, the cladding hoop stress σ_{ch} at the inner diameter of the cladding is used for the fracture mechanics calculation in Section 3. Also note that both Eqs. 4 and 6 can be reduced to pr_m/t for thin shell structures, where r_m is the mean radius of the cladding and t is the cladding wall thickness.

The stresses for the pellet are nor relevant in the present case, and therefore they are not calculated here. Nevertheless, it is interesting to note that the pellet hoop and radial stresses on the interface are both equal to the negative OPCI pressure (p).

2.2.2 Cladding Strains

On the cladding inner surface, a biaxial stress state exits because the axial loading of the fuel rod is not considered in the present case. By Hooke's law, the hoop (circumferential) strain ε_h is obtained as

$$\varepsilon_h = (\sigma_{ch} - \upsilon_0 \sigma_{cr})/E_o = (\sigma_{ch} + \upsilon_0 p)/E_o \tag{8}$$

In the case of uniform radial expansion, the hoop strain (ε_h) and radial strain (ε_r) are the same:

$$\varepsilon_r = \varepsilon_h \tag{9}$$

The radial strain of the cladding is sometimes denoted as (*ΔR/R*), where *R* represents the radius and *ΔR* is the increase of radius.

2.2.3 Young's Modulus of the Oxidizing Pellet (E_i)

In the calculation for press-fit pressure (p) with Eq. 3, the Young's modulus of the pellet (E_i) is needed. During the oxidation process, a series of conversion from UO_2 to U_3O_8 is taking place [e.g. 1-7]. Therefore, for different stage of the uranium oxides, the corresponding Young's modulus must be known for the calculation. The "rule of mixtures" developed for composite materials is adopted here:

$$E_i = (1-k)E_{UO2} + kE_{U3O8} \tag{10}$$

where E_{UO2} and E_{U3O8} are the Young's moduli of UO_2 and U_3O_8, respectively; and (1-k) and k are their volume fractions in the mixture (oxidizing pellet).

The Young's modulus E_{UO2} was given by Jiang and Wang [13] in their dynamic analysis of SNF system during transportation:

$$E_{UO2} = 201.3\ GPa \tag{11}$$

In a thin film experiment conducted by Lin et al. [14], different uranium oxide phases were obtained by controlling the oxygen in the total gas flow rate (f_{O2}) in the chamber. The Young's moduli for the cubic UO_2 film ($f_{O2} = 10\%$) and for the U_3O_8 thin films ($f_{O2} > 15\%$) were reported as 195 and 147 GPa, respectively. To be consistent with SNF analysis at Oak Ridge National Laboratory [10], the Young's modulus of U_3O_8 in the present work is estimated by scaling Eq 11 with the thin film results:

$$E_{U3O8} = E_{UO2} \times \frac{147\ GPa}{195\ GPa} = 151.8\ GPa \tag{12}$$

The Poisson's ratio of the pellet is not adjusted with the change of volume fraction, and $\nu_i = 0.32$ [13] is used throughout the calculation.

2.2.4 Estimation of Pellet Radial Growth (δ_R) due to Oxidation

To calculate the interface pressure (p) in Eq. 3, the radial growth of the pellet (δ_R) must be known. The parameter δ_R is defined as the difference between the oxidized pellet radius and its initial radius. Because it is assumed that the fuel-clad gap has been closed due to inservice thermal expansion and swelling of the fuel pellet, and the creepdown of cladding [7], the pellet is already in direct contact with the cladding before the fuel is taken out of service. Therefore, the initial pellet diameter is set to the inner diameter of the cladding in this analysis.

It is assumed that the as-manufactured pellet contains small fraction of porosity (denoted by ϕ). In the case of B&W 15 x 15 PWR fuel, for conservatism, $\phi = 5\%$ (based on the fuel pellet density equal to 95% TD [9]). For conservatism, the analysis also assumes that this void space remains unchanged during UO_2 conversion to U_3O_8 due to oxidation. For a given conversion fraction (k) from UO_2 to U_3O_8, the oxidized pellet volume (V) can be expressed by (see Appendix A)

$$V = V_0[1 + k(1 - \phi)(Q - 1)] \tag{13}$$

where V_0 is the initial volume of the pellet and

$$Q = \frac{\rho_{UO2} M_{U3O8}}{3(\rho_{U3O8} M_{UO2})} = 1.36443$$

In the above equation, ρ_{UO2} = 10.96 g/cm^3 is the density of UO_2, ρ_{U3O8} = 8.36 g/cm^3 is the density of U_3O_8, M_{UO2} = 270 g/mole is the molecular weight of UO_2, and M_{U3O8} = 842 g/mole is the molecular weight of U_3O_8.

Therefore, by denoting volume increase as $\Delta V = V - V_0$,

$$\frac{\Delta V}{V_0} = k(1 - \phi)(Q - 1) = 0.36443k(1 - \phi) \tag{14}$$

For simplicity, it is assumed that the pellet deformation is incompressible (conservation of volume) and that the axial direction of the pellet is constrained (i.e., no pellet length change during oxidation/swelling), the diametrical change can be expressed by

$$\frac{d}{d_0} = \sqrt{1 + \Delta V/V_0} \tag{15}$$

where d is the oxidized pellet diameter and d_0 is the initial diameter. The resulting radial growth of the pellet due to oxidation is

$$\delta_R = r_0\sqrt{1 + \Delta V/V_0} = r_0\sqrt{1 + k(1 - \phi)(Q - 1)} \tag{16}$$

where r_0 is the initial pellet radius prior to oxidation.

2.2.5 Cladding Stress Calculation Results

The analysis parameters and material properties are taken from Section 2:

(1) Cladding

Outer radius (fuel rod radius): R_{co}= 5.461 mm

Inner radius: R_{ci}= 4.788 mm

Cladding wall thickness: t= 0.673 mm

Young's modulus: E_o = 100 GPa (typical for high burn-up fuel)

Poisson's ration: ν_i= 0.37

(2) Pellet

Initial radius= cladding inner radius= 4.788 mm (assuming direct contact of pellet and cladding)

Young's modulus of UO_2: E_{UO2} = 201.3 GPa

Young's modulus of U_3O_8: E_{U3O8}= 151.8 GPa

Young's modulus of pellet: Use the rule of mixtures, Eq. 10

Poisson's ration ν_o= 0.32

(3) Pellet-Cladding Interface

Radial growth of the pellet due to oxidation: δ_R (Eq. 16)

Figure 3 shows the calculated OPCI pressure (press-fit) using Eq. 3 and the cladding hoop stress using Eq. (4). They are plotted as functions of the conversion fraction (k) from UO_2 to U_3O_8. For additional information, the diametrical change of the oxidized pellet (Eq. 15) is also plotted. The cladding hoop stress is the main input to calculate the stress intensity factor (K or K_I) and the crack opening area (COA).

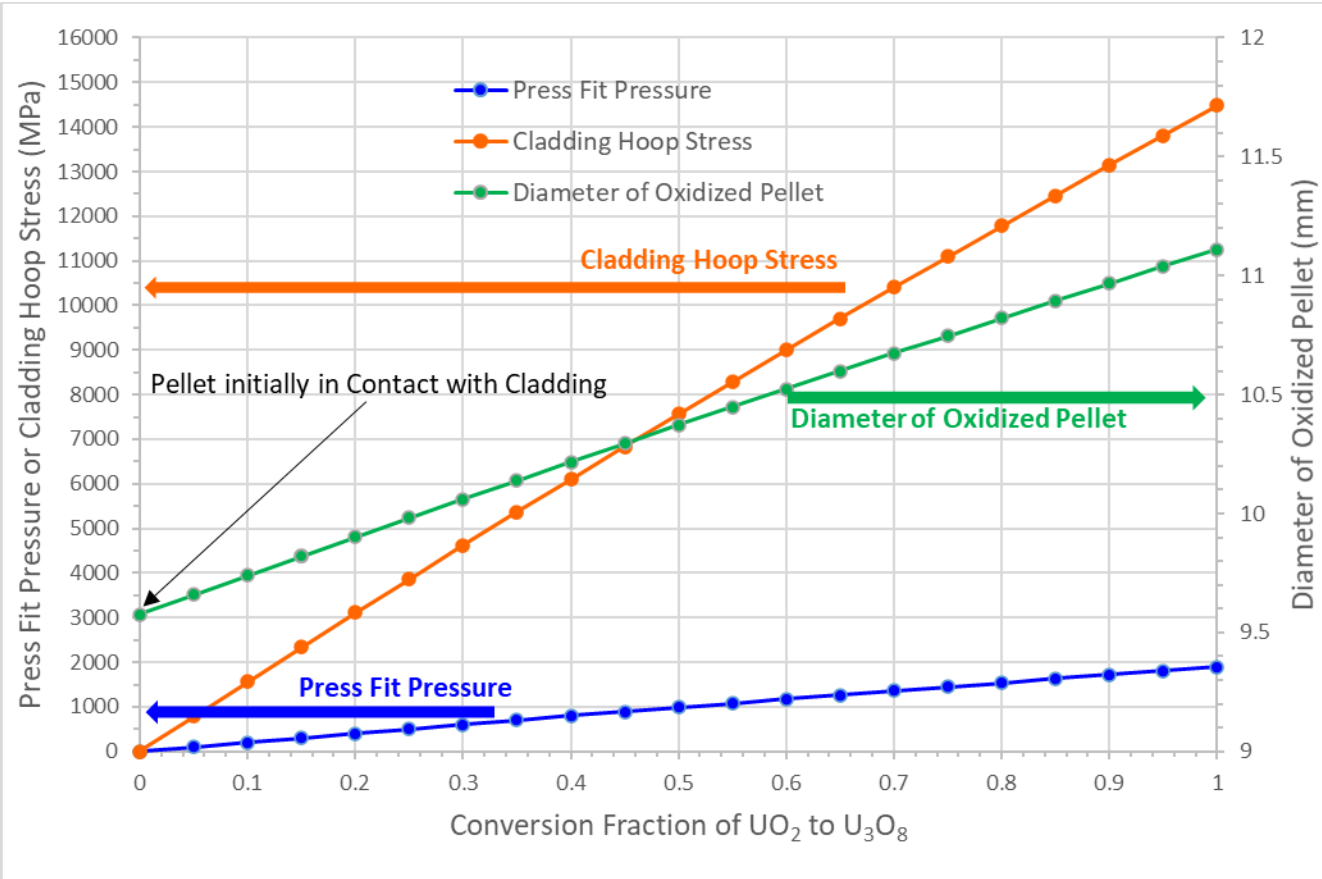


Figure 3. Cladding hoop stress and OPCI pressure vs. pellet UO_2 to U_3O_8 conversion fraction

3. FRACTURE ANALYSIS

Based on LEFM, the stress intensity factor (K) calculated from the applied load (in the present case, the cladding hoop stress) is compared to the fracture toughness (K_{IC}) of the cladding material (Zr-4). For a given hoop stress (Eq. 8), the crack length corresponds to $K = K_{IC}$ is defined as the critical crack length. This critical crack length is then used to calculate the critical COA.

3.1 Determination of Critical Crack Length

API 579 (2016) Annex 9B [12] is used to calculate the stress intensity factors at the crack tips of an axial through-wall crack in a cylinder (Fig. 4). Other stress intensity factor solutions [e.g., 15-20] can also be used, but API 579 appears to provide more conservative results, as documented in Appendix B.

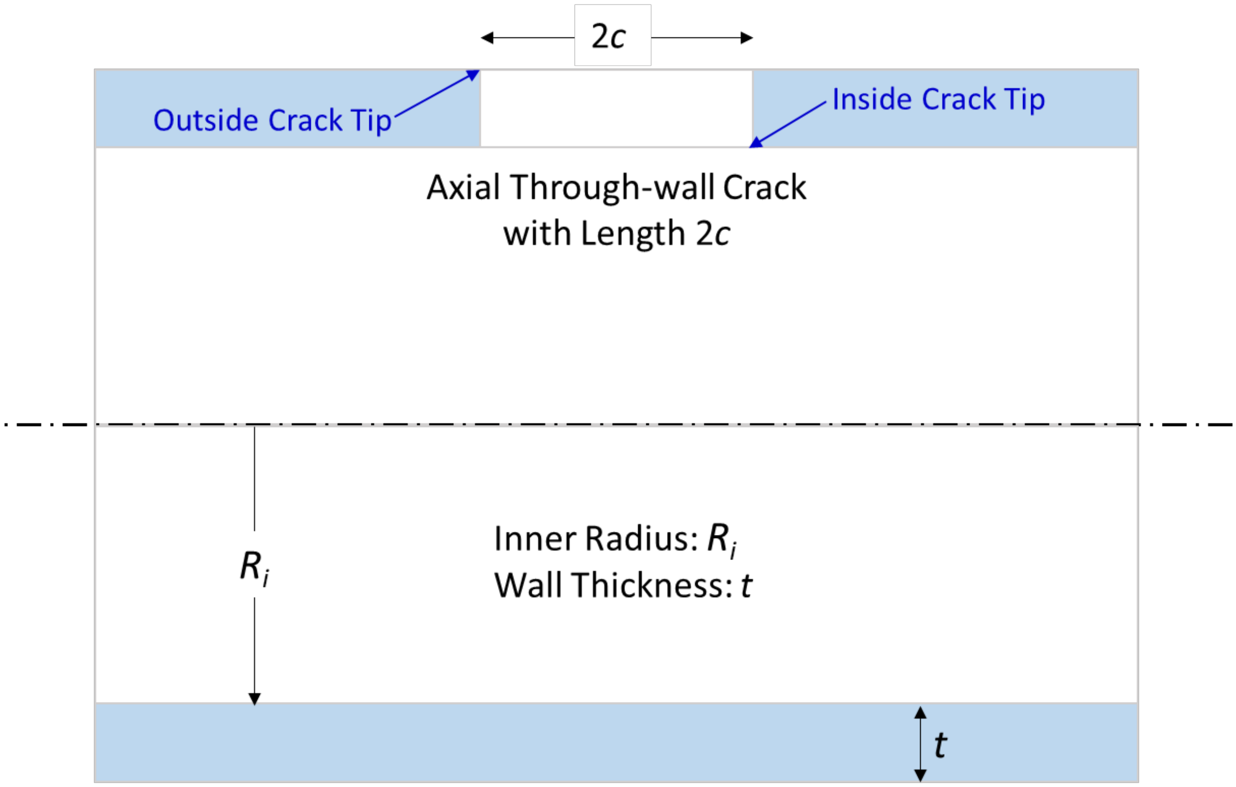


Figure 4. Sketch of an axial through-wall crack in a cylinder

In the API 579 formulation [12, Annex 9B], for a crack illustrated in Figure 4 is loaded with a membrane stress (σ_m) without bending, the stress intensity factor is

$$K_I = \sigma_m G_0 \sqrt{\pi c} \tag{17}$$

where G_0 is the influence coefficient and is expressed as

$$G_0 = \frac{A_0 + A_1\lambda + A_2\lambda^2 + A_3\lambda^3}{1 + A_4\lambda + A_5\lambda^2 + A_6\lambda^3} \tag{18}$$

and

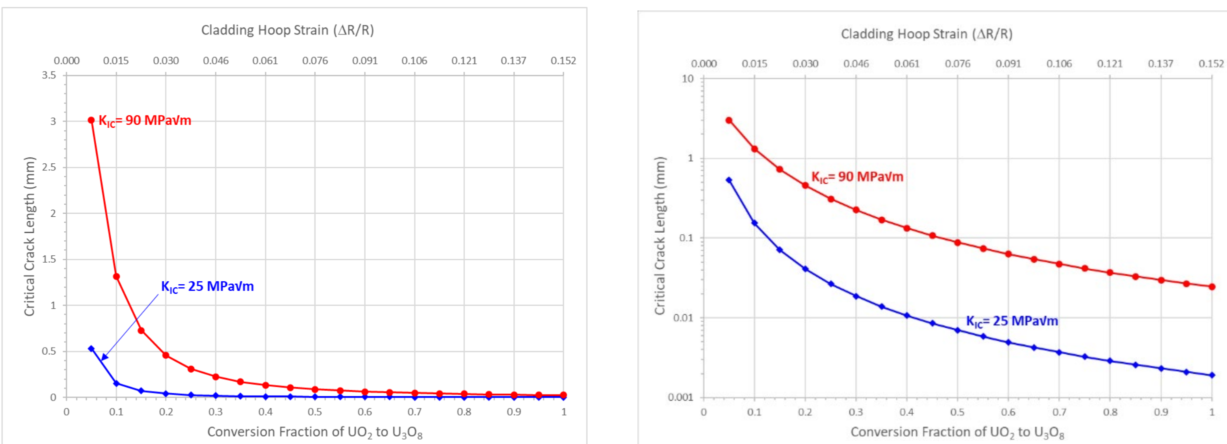
$$\lambda = \frac{1.818c}{R_i t} \tag{19}$$

For the fuel rod with the dimensions specified in Section 2.2.4 (R_{ci}= 4.788 mm), the wall thickness to inner radius ratio t/Ri is 0.1406. The constants A_i (i=1 to 6) in Eq. 18 can be obtained from API 579 and are listed in Table 1.

Table 1. Constants for Calculating Influence Coefficient G_0 for Evaluating Stress Intensity Factor

Crack Tip Location	For t/Ri = 0.1406 (by interpolation [12, Tables 9B.6 and 9B.7]) (Cladding Wall Thickness t = 0.673 mm and Fuel Inside Radius Ri = 4.788 mm)						
	A_0	A_1	A_2	A_3	A_4	A_5	A_6
Outside Surface	0.99497	0.54090	0.19590	0.00000	0.19393	0.03304	0.00009
Inside Surface	1.0070	0.1323	0.2375	0.0000	0.2506	0.0106	-0.0003

The fracture toughness (K_{IC}) of the cladding material must be known for the determination of the critical crack length. By reviewing the open literature, two K_{IC} values (25 and 90 MPa$\sqrt{m}$) [e.g. 21, 22] for Zr-4 are used to bound the analysis results. The critical crack length is plotted as a function of UO_2 to U_3O_8 conversion fraction and is shown in Figure 5. The corresponding cladding hoop strains (Eq. 8) can be seen from the secondary x-axis (i.e., top horizontal axis).



(a) **(b)**

Figure 5. Critical crack length vs. conversion fraction of uranium oxides and the cladding hoop strain in linear scale (a) and in semi-logarithmic scale (b)

3.2 Determination of Critical Crack Opening Area and Crack Opening Displacement

API 579 also provides the formula to calculate COA [12, Annex 9E]:

$$COA = \sigma_m H_0 \frac{2\pi c^2}{E} \tag{20}$$

where E is the Young's modulus of the material and H_0 is the influence coefficient and is defined as

$$H_0 = \frac{A_0 + A_1\lambda + A_2\lambda^2 + A_3\lambda^3}{1 + A_4\lambda + A_5\lambda^2 + A_6\lambda^3 + A_7\lambda^4} \tag{21}$$

Table 2 lists the constants A_i (i=0 to 7) for calculating COA with Eqs. 20 and 21; and λ has been defined in Eq. 19.

Table 2. Constants for Calculating Influence Coefficient H_0 for Evaluating Crack Opening Area

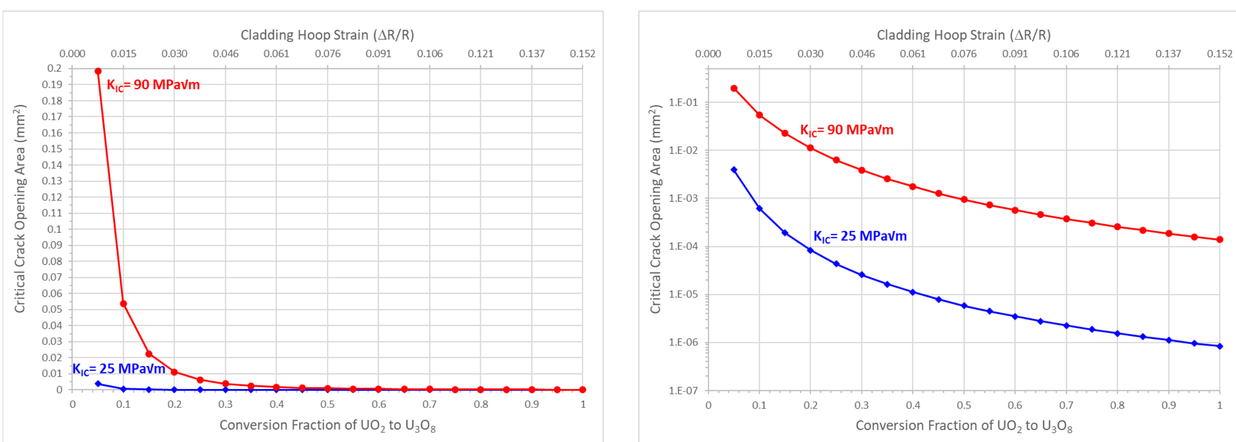
Crack Tip Location	For Ri/t = 7.1144 (by interpolation [12, Tables 9E.1 and 9E.2]) (Cladding Wall Thickness t = 0.673 mm and Fuel Inside Radius Ri = 4.788 mm)							
	A_0	A_1	A_2	A_3	A_4	A_5	A_6	A_7
Outside Surface	1.00550	0.59328	0.53049	0.52451	0.11531	0.82168	-0.07266	0.00271
Inside Surface	1.00892	-0.13133	0.21789	0.00000	0.04218	0.00615	-0.00031	0.00000

Note that the Young's modulus is needed for evaluating COA. In the present case, it is the Young's modulus of the cladding, which has been given in Section 2.2.5 (E_o = 100 GPa).

An approximate and convenient method to estimate the crack opening displacement is to assume that the deformed crack takes the form of an ellipse [e.g., 20, 23]. Therefore, crack opening displacement (COD) can be calculated by equating COA (Eq. 20) to the area of an ellipse πbc, where the equivalent crack opening displacement ($2b$) is the minor axis of this ellipse and its major axis 2c is the axial crack length (Fig. 4). Therefore,

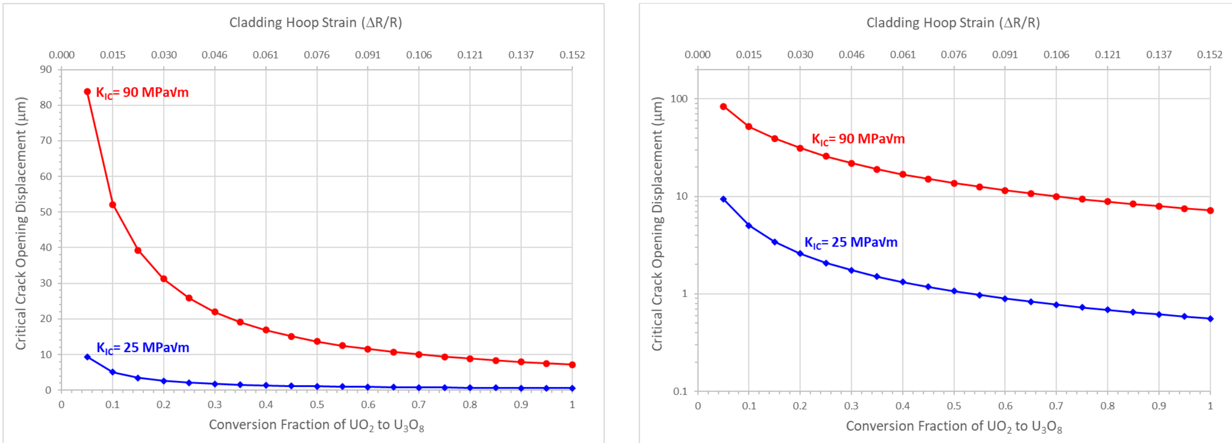
$$COD = 2b = 4cH_0\frac{\sigma_m}{E} \tag{22}$$

The calculated critical COA and COD are presented in Figures 6 and 7 as functions of conversion fraction (k) from UO_2 to U_3O_8. As in Figure 5, the corresponding cladding hoop strain can be read from the secondary x-axis (i.e., top horizontal axis).



(a) **(b)**

Figure 6. Critical crack opening area vs. conversion fraction of uranium oxides and the cladding hoop strain in linear scale (a) and in semi-logarithmic scale (b)



(a) **(b)**

Figure 7. Critical crack opening displacement vs. conversion fraction of uranium oxides and the cladding hoop strain in linear scale (a) and in semi-logarithmic scale (b)

4. CONCLUDING REMARKS

In the present work, Timoshenko solution [11] is first used to estimate the press-set pressure exerted by the oxidized pellet on the cladding. Based on the pressure, the stress in the cladding is obtained from the classic solution of a pressurized cylindrical structure; and the strain is calculated from linear elasticity (Hooke's law). This approach, along with the no-gap initial condition between the cladding and the pellet, inevitable leads to a very high stress state far exceeding the elastic limit of the cladding material. Therefore, the subsequent LEFM analysis results in a conservative (short) critical crack length with the corresponding critical crack opening area/displacement. For example, in the early stage of OPCI, when only 10% of UO_2 is converted to U_3O_8, the critical crack length is estimated as 0.15 mm for K_{IC} = 25 MPa√m and is 1.32 mm for K_{IC} =90 MPa√m, and the corresponding crack opening displacements are 5 μm and 52 μm, respectively - this small crack opening would preclude large-size pellet debris from leaving the rod.

The actual fracture toughness value of K_{IC} of a cladding at high burnup cladding conditions is to be determined, but values applied in this analysis are the best available. If the linear elastic deformation and fracture criterion approach needs to be relaxed to match the mechanical behavior, then elastic-plastic finite element analysis is recommended. It is highlighted that the sizes of the original artificial defects in the SNF experiment by Einziger and Strain (1986) [2] ranged from 8 to 760 μm, which are comparable to the present calculation results. Therefore, the small crack sizes as predicted from the present work could initiate crack propagation and could extend an initial breach in the fuel rod through pellet oxidation. Note that the smallest defect size (8 μm) in the experiment of Einziger and Strain was used to approximate the stress corrosion cracking-type cladding breach [2].

It is expected that the extent of growth from an unstable crack to a stable crack is limited by the extent of additional pellet oxidation and swelling along the length of the rod from the crack site. In other words, continued crack extension beyond only a local region of pellet oxidization would not occur due to removal of the displacement-based loading condition although the demonstration thereof was not possible with the present two-dimensional model in this analysis.[3]

The fracture toughness (K_{IC}) is a critical parameter to predict cladding failure. It is considered as a material property and must be determined experimentally. Work has been done in this area for decades [e.g. 24], but due to the complexity in zirconium alloy composition, irradiation history and environments, hydride orientation [25, 26], and test methods, etc., a more structured approach may be needed, as pointed out in the white paper by Sindelar, Louthan, and Hanson (2016) [27].

The fracture toughness of high burnup cladding has not been fully characterized. The testing may require additional considerations that include the radioactivity and material availability. Nontraditional test methods, such as the hot cell-ready, small specimen-oriented Spiral Notch Torsion Test (SNTT) developed at Oak Ridge National Laboratory [28, 29], may be one of the options. The companion advanced fracture mechanics and numerical methods may also need to be further developed to account for the unusual specimen shape and size in order to extract useful fracture parameters in consistent with the ASTM standard requirements.

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APPENDIX A: ESTIMATION OF FUEL PELLET VOLUME CHANGE DUE TO OXIDATION

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APPENDIX A

The equations used to estimate the oxidized pellet volume (Section 2.2.4) are derived in this appendix. With the initial pellet volume denoted as V_0, which may contain porosity [9] with void fraction ϕ, the volume initially occupied by UO_2 is $(1-\phi)V_0$.

The following parameters are defined for the analysis:

Density of UO_2: $\rho_{UO2} = 10.96\ g/cm^3$
Molecular weight of UO_2 $M_{UO2} = 238 + 16 \times 2 = 270\ g/mole$
Density of U_3O_8: $\rho_{U3O8} = 8.36\ g/cm^3$
Molecular weight of U_3O_8: $M_{U3O8} = 238 \times 3 + 16 \times 8 = 842\ g/mole$

As UO_2 is converting to U_3O_8 due to oxidation, the volume change can be estimated as follows:

Volume of UO_2 to be converted to U_3O_8 (before oxidation) = $k(1-\phi)V_0$

Weight of the UO_2 in the volume being converted to U_3O_8 = $k(1-\phi)V_0\,\rho_{UO2}$

Moles of UO_2 in the volume being converted to U_3O_8 = $\frac{k(1-\phi)V_0\,\rho_{UO2}}{M_{UO2}}$

After conversion:

Moles of U_3O_8 in the oxidized volume = $\frac{1}{3}\frac{k(1-\phi)V_0\,\rho_{UO2}}{M_{UO2}}$

Weight of U_3O_8 in the oxidized volume = $\frac{1}{3}\frac{k(1-\phi)V_0\,\rho_{UO2}\,M_{U3O8}}{M_{UO2}}$

Volume of U_3O_8 = $\frac{1}{3}\frac{k(1-\phi)V_0\,\rho_{UO2}\,M_{U3O8}}{M_{UO2}\,\rho_{U3O8}} = k(1-\phi)QV_0$

where $Q = \frac{\rho_{UO2}\,M_{U3O8}}{3M_{UO2}\,\rho_{U3O8}} = 1.36443$

<u>Calculation of Total Volume and Volume Change</u>

Assuming that the void space in the pellet (ϕV_0) remains unchanged, that is, no oxides will take up the volume of the voids, then the total pellet volume corresponding to conversion fraction k is

Total Volume = Volume of UO_2 + Volume of U_3O_8 + Volume of the voids (ϕV_0), or

$V = (1-k)(1-\phi)V_0 + k(1-\phi)QV_0 + \phi V_0$, or

$\frac{V}{V_0} = 1 + k(1-\phi)(Q-1) = 1 + 0.36443k(1-\phi)$

Define the volume increase as $\Delta V = V - V_0$, then

$\frac{\Delta V}{V_0} = k(1-\phi)(Q-1) = 0.36443k(1-\phi)$

Note that, if the pellet has no void space ($\phi = 0$) and if UO_2 is fully oxidized to U_3O_8 ($k = 1$), then

$$\Delta V = Q - 1 = 0.36443$$

which is the conversion limit or the maximum net volume expansion of the pellet (36% by volume) [30-32].

<u>Estimation of Oxidized Pellet Diameter</u>

Two assumptions are made to simplify the estimation for pellet diameter change resulting from oxidation:
(1) The axial direction of the pellet is constrained (i.e., no pellet length change during oxidation/swelling). The pellet length L_0 is a constant.
(2) The deformation is incompressible. The total volume is preserved (i.e., the pellet volume is unchanged before and after oxidation).

Denoting d_0 and d as the initial and final pellet diameter, respectively, and by the conservation of volume:

$$\frac{V}{V_0} = 1 + \frac{\Delta V}{V} = \frac{d^2}{d_0^2}$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}_0} = \sqrt{1 + \Delta \mathrm{V}/\mathrm{V}_0}$$

The above equations are used in Section 2.2.4 to estimate the pellet radial growth (δ_R) for cladding stress calculation in Section 2.2.1 (Timoshenko solution for press-fit [11]). The results are shown in Section 2.2.5 for the case of B&W 15 x 15 (PWR fuel assembly with 208 fuel rods [8]. The cladding hoop stress is used in Section 3 to calculate stress intensity factor (K) for a postulated flaw that might split the fuel rod due to pellet swelling from oxidation.

APPENDIX B: EVALUATION OF STRESS INTENSITY FACTOR CALCULATIONS

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APPENDIX B

Stress intensity factors and other fracture parameters can be calculated with many handbook and international consensus code solutions [e.g., 12, 17, 18]. In this appendix, the results from Tada, Paris, and Irwin [15] and from European structural integrity assessment procedure (SINTAP) [16, 17] are compared with API 579 [12] used in the main body of this report (Sections 3.1 and 3.2).

Only the case relevant to this report is investigated, that is, an axial through-wall crack in the fuel rod cladding subject to volume expansion of the fuel pellets due to oxidation that UO_2 is converted to U_3O_8.

The cladding deformation can be approximated by an axisymmetric condition. Under this simplification, the cladding hoop strain (ε_h) is expressed as (see Section 2):

$$\varepsilon_h = \Delta R/R$$

where R is the cladding mean radius and ΔR is the amount of cladding expansion in the radial direction. Instead of using a full field two-dimensional elastic solution (such as Eq. 8* in Section 2). A simple, uniaxial Hooke's law is used to calculate the hoop stress (σ_h) in the cladding with the Young's modulus E:

$$\sigma_h = E\varepsilon_h$$

The hoop stress (σ_h) is the main input to fracture analysis. Figure 4 shows the crack configuration. The formulations of Tada, et al. and SINTAP are described in Sections B1 and B2, respectively. The results are shown in Section B3.

B1 Tada, Paris, and Irwin Solution [15]

By Linear Elastic Fracture Mechanics (LEFM), the opening mode (Mode I) stress intensity factor (K_I) of a crack in the cladding longitudinal (axial) direction is

$$K_I = \sigma\sqrt{\pi c} \cdot F(\rho)$$

where c is the half crack length, σ is the tensile stress to open the crack ($\sigma = \sigma_h$ in the present case), $\rho = c/\sqrt{Rt}$, t is the cladding thickness, and the geometric-dependent function $F(\rho)$ is

$$F(\rho) = \sqrt{1 + 1.25\rho^2} \qquad \text{for } 0 < \rho \leq 1$$

$$F(\rho) = 0.6 + 0.9\rho \qquad \text{for } 1 \leq \rho \leq 5$$

The companion solution for the crack opening area (COA) and the geometry-dependent function $G(\rho)$ are

$$COA = \frac{\sigma}{E} 2\pi Rt \cdot G(\rho)$$

∗ Strictly speaking, Eq. 8 is only applied to the inner most element of the cladding where the press-fit pressure (p) is acting. Eq. 8 could be overly conservative to be applied to most part of the cladding.

$$G(\rho) = \lambda\rho^2 + 0.625\rho^4 \qquad \text{for } 0 < \rho \leq 1$$

$$G(\rho) = 0.14 + 0.36\lambda\rho^2 + 0.72\rho^3 + 0.405\rho^4 \qquad \text{for } 1 \leq \rho \leq 5$$

B2 SINTAP Solution

The stress intensity factor formula proposed by the Structural INTegrity Assessment Procedures (SINTAP) for European Industry [17] is similar to that reported by Tada, et al. (Section B1). However, SINTAP equations are given for both crack tips - on the internal surface (K_{in}) and on the external surface (K_{out}), as depicted in Figure 4. In the case of no bending stress, the stress intensity factor solutions are written as

$$K_{in} = \sigma\sqrt{\pi c}\,(G1(\rho) - g1(\rho))$$

$$K_{out} = \sigma\sqrt{\pi c}\,\left(G1(\rho) + g1(\rho)\right)$$

where

$$\rho = c/\sqrt{Rt}$$

$$G1(\rho) = \sqrt{1 + 0.7044\rho + 0.8378\rho^2}$$

and

$$g1(\rho) = -0.035211 + 0.39394\rho - 0.20036\rho^2 + 0.028085\rho^3 - 0.0018763\rho^4 + \frac{\left(3.912 - \ln\left(\frac{R}{t}\right)\right)}{1.6094}(0.01556 - 0.05202\rho + 0.0381\rho^2 - 0.012782\rho^3 + 0.001246\rho^4)$$

The range of applicability is $0 \leq \rho \leq 4.4$.

Without considering the crack face plasticity effect, the crack opening area, *COA*, is expressed as [17, 19, 20]

$$COA = \Upsilon(\omega)\frac{2\pi c^2\sigma}{E}$$

$$\Upsilon(\omega) = 1 + 0.1\omega + 0.16\omega^2$$

$$\omega^4 = 12(1 - \upsilon^2)\frac{c^4}{R^2t^2}$$

These equations are also adopted by British Standard (BS-7910 [18]).

B3 Comparison of Critical Crack Length and Crack Opening Area from Various Formulations

Given two bounding fracture toughness values (K_{IC} = 25 and 90 MPa√m), the critical crack lengths are calculated for the hoop strains (which are proportional to the hoop stresses) by Tada et al. (Section B1), SINTAP (Section B2), and API 579 (Section 3.1 [12]). The results are shown in Figure B1. Similarly, the crack opening areas are obtained and shown in Figure B2. It can be seen that the API 579 formulation consistently gives more conservative results. That is, for a given cladding hoop stress or strain, API 579 predicts lowest values for critical crack length and crack opening area. Therefore, API 579 is chosen for the full fracture analysis in Section 3 of the report. However, the results also show that SINTAP solutions for both critical crack length and opening area are very close to those determined with API 579 procedure, at least for the present calculation range. Therefore, if a quick assessment is needed, the SINTAP formulation (Section B2) may be considered. Note that some SINTAP procedures are consistent with the British Standards (BS-7910 [16-19]). On the other hand, the equations provided by Tada et al. [15] are the easiest to use (Sections B1), but might contain small but sometimes acceptable errors due to simplification.

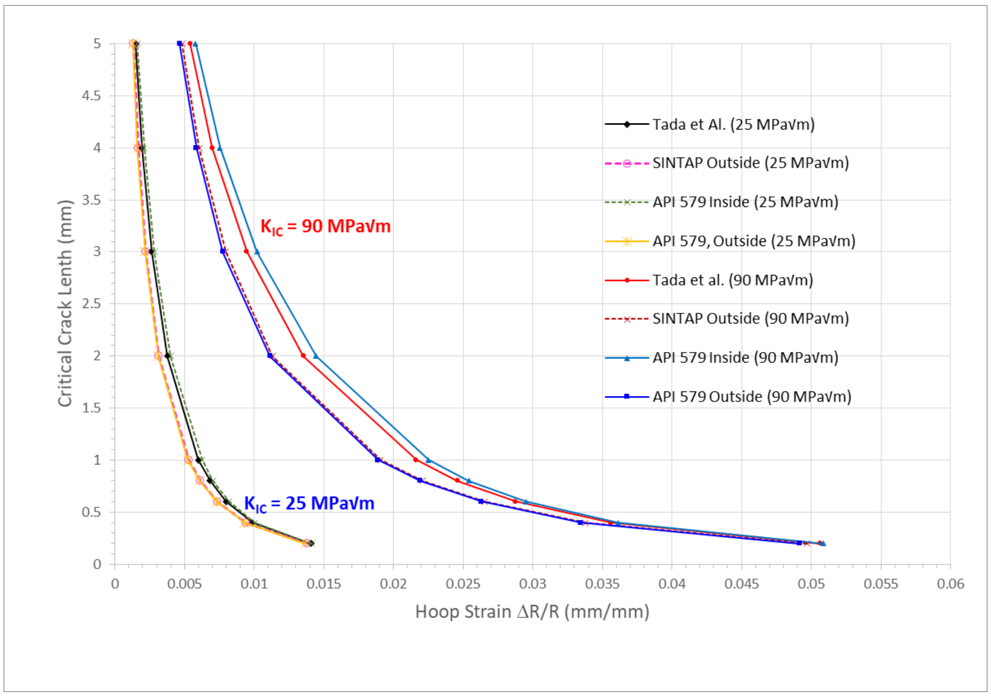

Figure B-1. Comparison of critical crack lengths calculated by Tada, et al. [15], SINTAP [17], and API 579 [12]

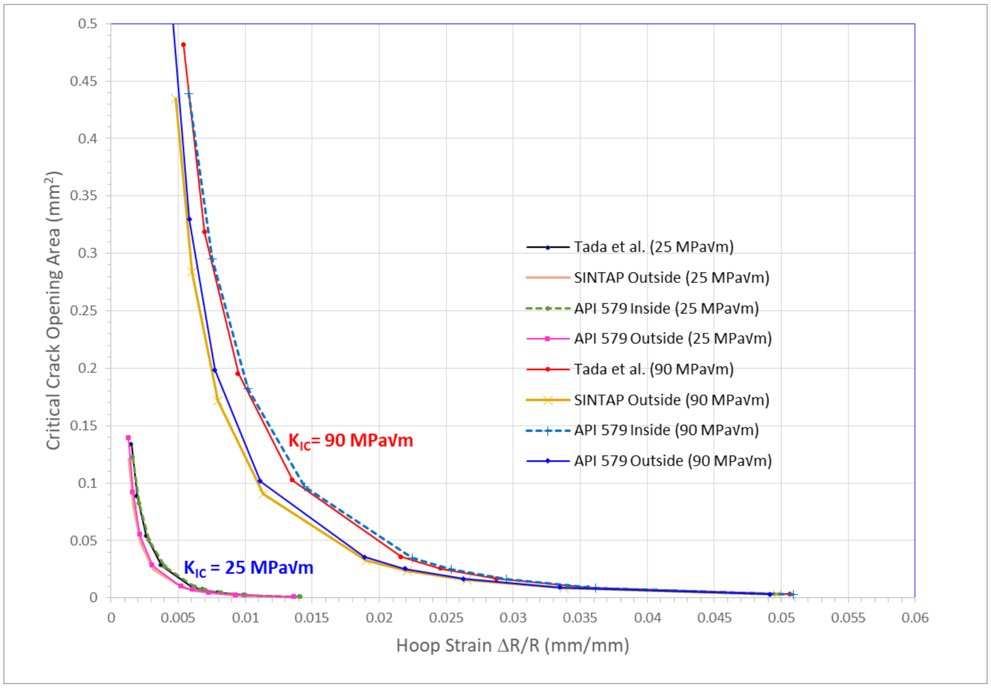

Figure B-2. Comparison of critical crack opening areas calculated by Tada, et al. [15], SINTAP [17], and API 579 [12]