

Model Support for an Out-Reactor-Instrumented-Defected-Fuel-Experiment to Validate the RMC Fuel Oxidation Model

A.D. Quastel¹, E.C. Corcoran¹, B.J. Lewis¹, C. Thiriet², and G. Hadaller³

¹Chemistry and Chemical Engineering Department, Royal Military College of Canada, P.O. Box 17000 Station Forces, Kingston, Ontario, Canada, K7K7B4

²Atomic Energy of Canada Limited, Chalk River Laboratories, Chalk River, Ontario, Canada, K0J1J0

³Stern Laboratories Inc., 1590 Burlington Street East, Hamilton, Ontario, Canada, L8H3L3

Abstract

An out-reactor fuel oxidation experiment with controlled parameters is being planned to provide data for validation of the Royal Military College (RMC) mechanistic fuel oxidation model. In support of this work, fuel oxidation 2D $r-\theta$ and 3D models are presented. The 2D $r-\theta$ model with radial cracks provides the radial temperature distribution in the test fuel element and also provides heating power information. The 3D model with radial cracks and a pellet-pellet gap under a defected sheath indicate that an oxygen stoichiometry deviation of 0.057 could result within one week of heating a defected UO_2 fuel element with a 5-mm² sheath defect.

1. Introduction

A mechanistic fuel oxidation model for defective fuel has been developed at the Royal Military College of Canada (RMC) [1] but a controlled experiment has yet to be performed to validate and possibly improve the model. The fuel element Zircaloy sheathing in CANDU fuel prevents the release of fission products into the coolant and protects the fuel from being oxidized. On rare occasions, a small hole or crack can occur in the sheathing during reactor operation as a result of debris fretting, pellet-cladding interaction or manufacture defects. Such sheath breaches allow coolant (heavy water) to enter the fuel element and make direct contact with the fuel [2,3] leading to fuel oxidation. As the fuel is oxidized, the fuel thermal conductivity will be degraded resulting in higher fuel temperatures. Moreover, in hyper-stoichiometric fuel, the melting temperature will be reduced leading possibly to centreline fuel melting in high-powered elements, particularly during accident conditions [4-7]. Fission product release will also be enhanced by a greater mobility in the hyper-stoichiometric fuel [8].

The fuel oxidation model has been extended to help design an out-reactor test. This test can be eventually used for model validation. An Out-Reactor Instrumented Defective Fuel Experiment currently is therefore being planned by AECL-CRL (Atomic Energy of Canada Limited - Chalk River Laboratories) at the STERN Laboratories to measure, in real-time, the fuel element temperature at various radial and axial locations. As mentioned the out-reactor test will provide important data for the validation of the RMC defective fuel oxidation model.

Other experiments have been conducted previously to investigate various aspects of defective fuel behaviour. Lewis *et al* [3] and Hüttig *et al* [9] investigated fission product release, Une *et al* [10] measured post irradiation fuel oxidation, Limbäck *et al* [11] and Cheng *et al* [12] investigated secondary fuel degradation with in-situ centreline fuel temperature measurements and hydrogen gas pressure measurements in the later experiment. The motivation for the proposed experiment is that fuel oxidation has never been investigated experimentally at both high coolant pressure (~10 MPa) and reactor temperatures while simultaneously measuring in-situ fuel temperatures (and hence thermal conductivity). The proposed experiment would also incorporate highly controlled test parameters such as the onset of a sheath defect (of a specific size), heating duration and power settings. The test results would help benchmark the RMC fuel oxidation model. The model could then be incorporated into fuel performance codes for defective fuel assessment [13]. An experimentally demonstrated fuel oxidation model is applicable not only to CANDU reactors but also to PWRs and BWRs, which constitute about 75% of all world power reactors.

This paper provides 2D r - θ and 3D fuel oxidation modelling results in support of an out-reactor fuel oxidation experiment. Included in this paper are model results for oxidation that occurs in specifically defined radial fuel cracks where it is believed increased oxidation occurs as well as oxidation that may occur in a pellet-pellet interface gap near the defect site in the sheath.

2. Proposed out-reactor-instrumented-defective-fuel-experiment setup

The out-reactor test facility at STERN Laboratories will include a small self-contained coolant loop capable of operating at CANDU reactor conditions. This loop is designed to run at up to 10 MPa inlet pressure and a normal coolant temperatures to 310°C. A laboratory data acquisition system will monitor the loop and test-fuel simulator instrumentation.

A fuel element would have 31 fuel pellets with an axial clearance of 1 to 3 mm. Typical fuel sheath defect surface areas have been observed from < 1 to 13 mm² [7,14]. At a chosen time after a conditioning heating period, an artificial slit defect will be initiated in-situ in the sheath. The breached sheath will expose the fuel to water at a temperature of approximately 300°C and a pressure of approximately 10 MPa.

Each test pellet will be about 16-mm in length and 12-mm in diameter. The test pellets will include a central hole to accommodate an electrical heating element. Temperature measurement of the test fuel will be performed in real time with thermocouples at three radial positions in the test pellet as indicated in Figure 1.

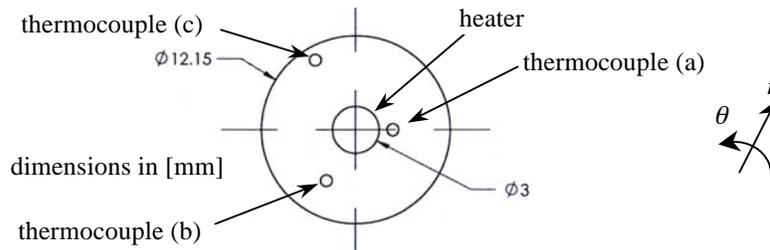


Figure 1: Radial cross section of planned test pellet with drill holes. The 3-mm diameter central hole is for the electrical heating wire. The smaller holes provide access for thermocouples and thermocouple wires. Thermocouple sites at: a) close to the pellet centre and near the heating element, (b) between the pellet centre and pellet outer surface and (c) near the outer surface of the pellet.

An electrical heating wire will run through the entire central length of the test fuel element. This heating technique has been successfully employed in the past by Oguma [15] in fuel pellets. The heater element wire will be approximately 3-mm in diameter. Iridium (Ir) has been chosen for making the wire since it is a noble metal and has a high melting temperature (2466°C). In order to prevent electric arcing between the heating element wire and the fuel pellets, the Zircaloy sheathing will be connected in parallel to the Ir wire conductor.

Post experiment measurement of the oxygen potential, or the O/M ratio, at several radial locations in the test fuel pellet will be required for validating the fuel oxidation model. The first method (a macroscopic approach) is the Coulometric Titration (CT) method [14] employed previously at AECL-CRL to measure the average O/M ratio of spent CANDU fuel, which has a sensitivity of $x = 0.01$ in UO_{2+x} . The second method (a microscopic approach) uses Wavelength Dispersive Spectroscopy (WDS) with X-ray diffraction (XRD) [16] to assess local oxygen concentrations. Preliminary tests will be performed to estimate the measurement sensitivity.

3. Fuel oxidation model theory

The model used to produce results presented in this paper is based on the conceptual model of Higgs [1,17]. The model describes the fuel oxidation processes that occur within a defective fuel element operating under normal conditions. The model was modified for the current study to represent an inner-surface heated and unirradiated fuel element in the out-reactor experiment. The model was also modified to include specifically defined radial fuel cracks and a pellet-pellet gap. The model consists of a heat conduction equation, a gas transport equation and an oxygen diffusion transport equation, all coupled together as discussed in the following section.

3.1 Mechanistic fuel oxidation model

In the mechanistic model [1] a treatment is required for both gas phase and solid-state diffusion, which are controlled by temperature-dependent reactions. This necessitates knowledge of the temperature distribution in the fuel element. Hydrogen (H_2) and steam (H_2O) are specifically considered in this treatment rather than deuterium and heavy water.

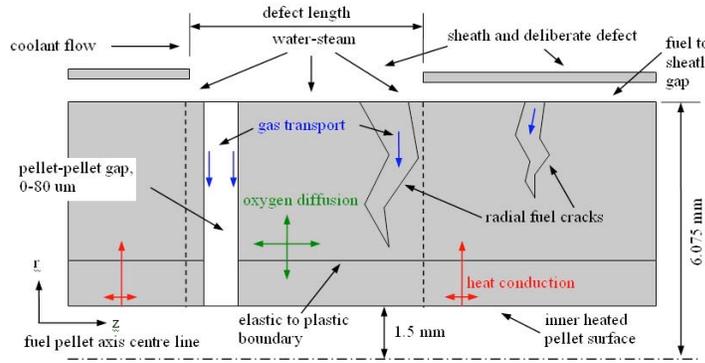


Figure 2: A 2D z - r representation of test fuel pellet. Heat conduction, gas transport in cracks and pellet-pellet gap and oxygen diffusion in the fuel are modelled. The defect width, not shown, is 1-mm.

Figure 2 depicts an axial cross section of a test fuel element. Fuel cracks that will appear in the fuel pellets are a result of fuel thermal expansion [15,18], and is an important model parameter. Below the elastic-plastic boundary, cracks will initially appear but will later self heal [19,20]. The temperature at which this transition occurs in the model is 1523 K, though in reality it occurs over a range of temperatures [15,20]. Figure 2 depicts a deliberate sheath defect which is 1-mm wide (into the page) and 5-20 mm long in the axial z -direction. Elevated oxidation occurs when the coolant steam makes contact with the hotter regions of the fuel, via the cracks and the pellet-pellet gap.

The initial hydrogen molar fraction, q , at the defect location and in the volume of the radial cracks directly under the defect site, is assumed to be 4.1×10^{-6} moles m^{-3} . This value is the hydrogen mole fraction of the coolant in reactor [1] and is used in the current model.

The generalized mass balance equation for oxygen transport in the fuel matrix is given by Eq. 1,

$$c_u \frac{\partial x}{\partial t} = c_u \nabla \cdot \left(D \left(\nabla x + x \frac{Q}{RT^2} \nabla T \right) \right) + R_f^{react} \quad (1)$$

where

$$D = 2.5 \times 10^{-4} \cdot \exp(-16400/T) \text{ m}^2 \text{ s}^{-1} \quad (2)$$

and x is the oxygen deviation from stoichiometry in the uranium oxide matrix (UO_{2+x}), c_u is the molar density of uranium, R is the universal gas constant, T (in K) is temperature. R_f^{react} is the rate of reaction for either fuel oxidation or reduction in moles O or H_2 $m^{-2} s^{-1}$. D in Eq. 2 is the diffusion coefficient for oxygen interstitials, which is a function of temperature (T in K) [1]. Q is the molar effective heat transport given by Eq. 3, (where x is the stoichiometric deviation value). A Neumann boundary condition for the oxygen stoichiometric deviation is taken as zero at all external geometric boundaries.

$$Q = -3.5 \times 10^{34} \exp(-17(4 + 2x)) \text{ J mol}^{-1} \quad (3)$$

The kinetic reaction rate R_f^{react} in Eq. (1) for fuel oxidation is given by Eq. 4:

$$R_f^{react} = c_u \alpha \sqrt{(1-q)p_t} (x_e - x) \quad (4)$$

where α is the rate coefficient for the surface-exchange of oxygen ($\alpha = 0.365 \exp(-23500/T)$ (K)) m s^{-1} [1]). At the pellet surface p_t is the total system pressure in atmospheres, q is the hydrogen mole fraction, x (or X_{dev}) is stoichiometric deviation, and x_e is the equilibrium stoichiometry deviation based on the local oxygen potential of the gas in the fuel cracks [1].

Hydrogen is contributed to the gas environment in the fuel cracks by the fuel-oxidation reaction. The mass balance for the hydrogen molar concentration, qc_g , in the fuel cracks is given in general form by Eq. 5 where c_g is the total molar concentration

$$c_g \frac{dq}{dt} = \nabla \cdot (c_g D_g \nabla q) + R_f^{react} \quad (5)$$

of gas in mol m^{-3} and $c_g D_g$ is the steam diffusivity quantity in $\text{mol m}^{-1} \text{s}^{-1}$. Eq. 5 is applicable only in the domain above the elastic-plastic boundary (see Figure 2) and in the fuel cracks and pellet-pellet gap. The temperature profile in the fuel element is obtained from the solution of the general time-dependent heat conduction equation, Eq. 6,

$$\rho_s C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q_v \quad (6)$$

where ρ_s is the fuel density, C_p is the specific heat of the fuel, k is the thermal conductivity of the fuel and Q_v is the volumetric heat source term of the nuclear fuel. In the current 2D r - θ model, the Q_v term is the ohmic heating generated in the iridium wire and Zircaloy sheath and to a small extent in the UO_2 fuel. In the 3D model, this term is set to zero and replaced by temperature boundary conditions. C_p and k are both functions of T and x .

It is worth noting here that in the previous Higgs model [1] the coefficients α_f and ε , which were the pellet crack surface area to fuel volume ratio and the volume of cracks to the volume of fuel ratio, were used in Eqs. 1 and 5. This was done since these model parameters were averaged over the model domains. In the current models, radial cracks are specifically modelled so these coefficients are not used.

3.2 The 2D r - θ and the 3D fuel oxidation model

In this paper, the fuel oxidation model is solved in both 2D r - θ and 3D geometries. The 2D r - θ geometry is less computationally expensive; however this representation tends to over-predict the extent of fuel oxidation as the defect length is not specified (i.e. the defect length is as long as the entire model). The 3D geometry is more computationally expensive but represents the extent of fuel oxidation for the actual size of the defect. In Figure 3 (a), the green area on the sheath represents a continuous slit defect along the axis of the fuel element in the 2D r - θ model. The yellow area is a true representation of the sheath defect in the 3D model. The presented models consider only radial fuel cracks since they are the most prevalent and are believed to provide the best path for gas transport, though azimuthal and axial cracks will also be present, see Figure 3 (b), which defines the different cracks.

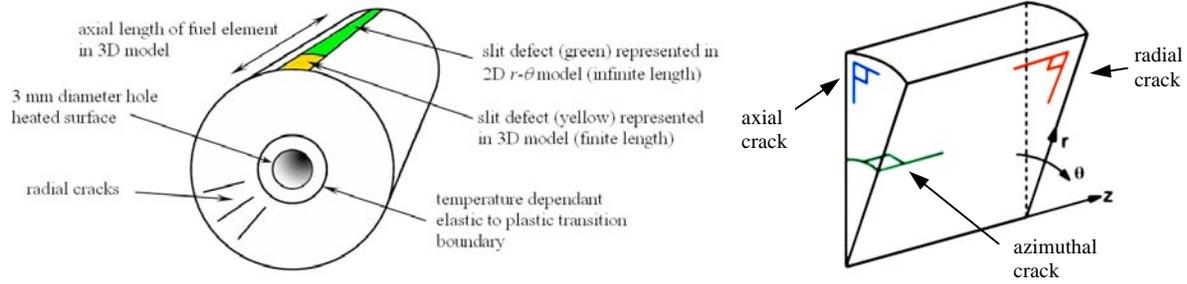


Figure 3: (a) 3D and 2D r - θ model defect representations; the green area represents an infinite length sheath defect in a 2D model and the yellow area represents a finite length defect in the 3D model and (b) different possible fuel crack orientations.

In the 3D model, the oxygen transport in the solid fuel matrix occurs in all directions (though it is dominant in the radial direction due to the high temperature gradient), so Eq. 1 becomes:

$$c_c \frac{\partial x}{\partial t} = c_c \left[\frac{1}{r} \frac{\partial}{\partial r} \left(rD \left(\frac{\partial x}{\partial r} + x \frac{Q}{RT^2} \frac{\partial T}{\partial r} \right) \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left(D \left(\frac{1}{r} \frac{\partial x}{\partial \theta} + x \frac{Q}{RT^2} \frac{1}{r} \frac{\partial T}{\partial \theta} \right) \right) + \frac{\partial}{\partial z} \left(D \left(\frac{\partial x}{\partial z} + x \frac{Q}{RT^2} \frac{\partial T}{\partial z} \right) \right) \right] + R_f^{react} \quad (7)$$

In the 2D r - θ model Eq. 7 simplifies by removing the third, z coordinate, term. Also, if temperature is independent of θ then the second term could also be neglected. But, in reality, the θ term will not cancel out in the vicinity of thermocouples and thermocouple drilled-holes, nor will the z term when consideration is made of the varying fuel thermal conductivity that is dependent on the degree of fuel oxidation.

Hydrogen gas diffusion in the radial fuel cracks and in the fuel-to-sheath gap is considered in the radial and azimuthal directions in the 2D r - θ model. Thus the differential equation for the hydrogen mole fraction q (Eq. 5) in the cracked UO_2 solid becomes:

$$c_g \frac{\partial q}{\partial t} = \frac{1}{\tau^2 r} \left[\frac{\partial}{\partial r} \left(r c_g D_g \frac{\partial q}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\frac{c_g D_g}{r} \frac{\partial q}{\partial \theta} \right) \right] + R_f^{react} \quad (8)$$

where t is time and τ is path tortuosity and the z -polar component is neglected.

The heat equation (Eq. 6) in the 3D becomes:

$$\rho_s C_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left(\frac{k}{r} \frac{\partial T}{\partial \theta} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + Q_v \quad (9)$$

In the 2D r - θ model, the heat equation simplifies by removing the z -polar coordinate term and in the 3D model the heat source term is removed and replaced with a temperature boundary condition at the heater surface.

3.3 Fuel-to-sheath gap thermal conductivity treatment

In the out-reactor fuel oxidation experiment, the intent is to simulate the condition of the fuel element before the Zircaloy sheath is defected to start the oxidation experiment. CANDU fuel sheath thickness is 0.4 mm thick [2,21] and because of fuel thermal expansion and cladding creepdown due to coolant pressure the fuel-to-sheath gap will close. When the gap closes heat will be transported by conduction where there is physical contact and by heat conduction via the

gas film that fills the portion of the interface where contact is not made [20]. Considering surface roughness the heat transfer coefficients for these two mediums are:

$$h_{solid} = \frac{k_m P_i^{1/2}}{a_0 R_{rms}^{1/2} H} \quad (10)$$

$$h_{gas} = \frac{k_f}{1.5(R_1 + R_2) + t_g + g \left(\frac{T_{gap}}{273} \right)^{2.405} (0.101/P_{gap})} \quad (11)$$

where $a_0 = 8.6 \times 10^{-3} \text{ m}^{0.5} \text{ MPa}^{-0.5}$, k_m and k_f are the harmonic mean thermal conductivity of the solids and the thermal conductivity of the gas in the gap, respectively, $P_i = Y_s t_s / r_{si}$ is the interfacial pressure between the fuel and the sheath surfaces (MPa),

$R_{rms} = \sqrt{(R_1^2 + R_2^2)/2} = 0.8 \mu\text{m}$ is the root-mean-square roughness of the fuel pellet and sheathing surfaces, R_1 and R_2 , and $H = 4.4 Y_s$ is the Meyer hardness of the Zircaloy sheath (MPa) as a function of the yield strength of the sheath Y_s which is $297.39 - 0.2733 * T_{sheath_ave}$ where the average temperature of the sheath is in (K). The terms t_s and r_{si} refer to the sheath thickness, and inner its radius, respectively, t_g is the gap thickness, g is the temperature jump distance for steam in (m) [2], and T_{gap} and P_{gap} are the average gap temperature and pressure, respectively [22,23]. With these calculated values an effective thermal conductivity value is derived and is applied in the fuel-to-sheath gap.

$$\frac{h_{solid} + h_{gas}}{h_{gas}} k_{gas} = k_{gap_effective} \quad (12)$$

3.4 Flux terms used at fuel crack and gas domain interfaces

The interaction of the steam (or gas) and the cracked fuel occurs at the gas-to-fuel interfaces, which is an example of a heterogeneous (gas to solid) chemical reaction [24]. In the current models, the oxygen diffusion equation, Eq. 1, and the gas diffusion equation, Eq. 5, occur in separate domains where the source term, R_f^{react} , takes a value of zero. Nevertheless $R_f^{react}(x, q)$ can be expressed so that Eqs. 1 and 5 are coupled together at the fuel-to-gas (steam) interfaces. This is accomplished in Comsol Multiphysics using flux terms at domain common boundaries. Table 1 give the flux terms for the two coupled equations.

Table 1: Flux term definitions at gas-to-fuel surface boundaries

Equation	Inward flux term	Equivalent weak form [25] term
Oxygen diffusion equation, Eq. 1	$R_f^{react} \frac{1}{c_u}$	$x_{dev_test} R_f^{react} \frac{1}{c_u}$
Gas diffusion equation, Eq. 5	R_f^{react}	$q_{test} R_f^{react}$

The equivalent weak form terms are also provided in the table and can be used in the weak form Comsol entry instead of the flux terms to yield the same numeric result. The weak form is discussed by Zimmerman [25].

4. Model results and discussion

The model equations discussed in Section 3 are solved with COMSOL Multiphysics software [26]. Two time dependent models are presented: A 2D r - θ model and a 3D model. Although steady state results are not fully achieved in two weeks, this period of time is considered an optimistic upper limit for the lifespan of the heater element in the planned experiment.

4.1 2D r - θ Radial model results

The fuel oxidation model was applied in a 2D r - θ model (a fuel element cross section). Included in the model are the temperature dependant thermal conductivity properties of the central iridium heater wire, the three different thermocouple materials, the gas (steam), the uranium dioxide fuel and the Zircaloy sheath. Figure 4 depicts the locations of the heater element, the radial cracks, the thermocouples, the defected sheath and the model meshing. The sheath defect is 1-mm wide. The crack depth was preset to where the temperature in the fuel was near 1523K (after one day of modelled time). The crack width was set to 15 μm with reference to work by Williford [27]. The fuel-to-sheath gap was set to 1 μm to be in line with the root-mean-square roughness of the pellet surface and the sheathing inner surface.

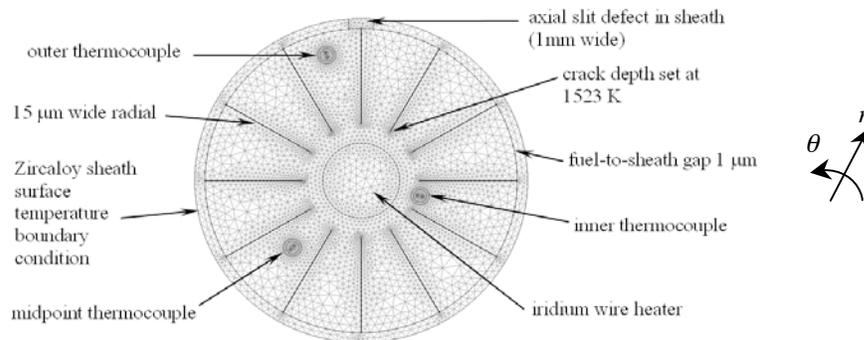


Figure 4: Cross section of fuel element with a defected sheath, thermocouples and heater element.

The model was run for a heating time of two weeks. The Zircaloy sheath surface temperature was set to 300°C. Electrical heating was used to heat the fuel element, specifically ohmic heating was modelled in the iridium wire, the UO_2 fuel and the Zircaloy sheathing. A current divider was included to calculate the current running through each material in the parallel circuit and each electrical resistance was calculated using an electrical conductivity equation, where the resistivity of each material is $\rho(T)$. From this the power (T) [kW m^{-3}] of each material domain was calculated and used for the source term in Eq. 6. The number of radial cracks was chosen to be the linear power [kW m^{-1}] of the iridium wire divided by two. This follows the work by Higgs [1] and Oguma [15]. The power generated in the sheathing is expected to be mostly dissipated in the coolant so it is not expected to contribute to the radial crack number formation. The tortuosity factor τ of the radial cracks was set to 1 but it is reasonable to assume that it will be greater than 1 since the cracks are not perfectly straight. A τ value greater than 1 tends to reduce fuel oxidation in the 2D r - θ model.

The temperature distribution and oxygen stoichiometric deviation (X_{dev}) predictions using the 2D r - θ model, after 2 weeks of heating, are shown in Figure 5 (a) and (b), respectively. The azimuthal variation in the temperature and X_{dev} distribution can be observed in the 2D plots.

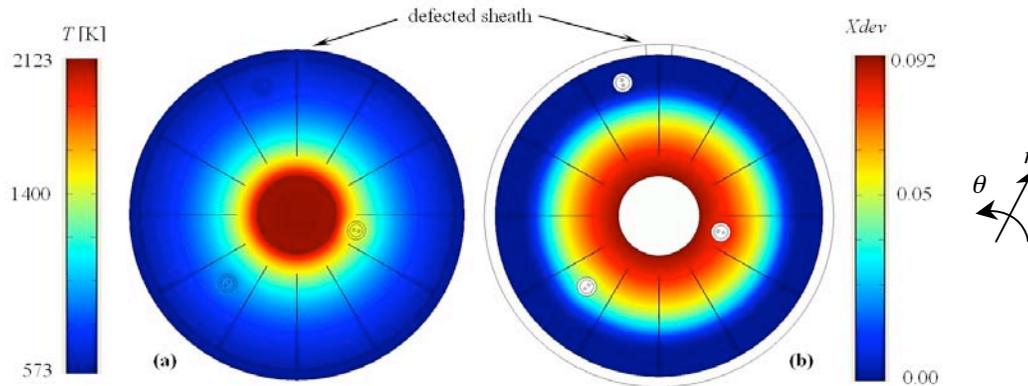


Figure 5: (a) Temperature distribution and (b) oxygen stoichiometric deviation distribution in the UO_2 fuel element for a 2-week heating time.

The total current input in the model was set to 1266 amps. The resulting linear power to attain the temperature at the interface of the heating element and inner surface of UO_2 pellets was 23 kW m^{-1} assuming that a direct current is used. The model showed that the current flowing through the iridium wire was ~ 563 amps, through the Zircaloy sheath was ~ 703 amps and through the UO_2 was fuel was 0.15 amps. Table 2 provides the maximum oxygen stoichiometric deviation in the fuel element using the 2D r - θ model.

Table 2: Inner surface temperature, required heater power and corresponding maximum oxygen stoichiometric deviation results using a 2D r - θ model, using an iridium wire heater.

Model	Temperature at inner surface of UO_2 pellet (1.5-mm radius) [$^{\circ}C$]	Power applied in iridium wire conductor [$\text{kW}\cdot\text{m}^{-1}$]	Maximum oxygen stoichiometric deviation in UO_{2+x} test fuel element	
			1 week of heating time	2 weeks of heating time
2D r - θ	1845	~ 23	0.081	0.092

The results presented in Table 2 assume a full length slit defect using the 2D r - θ model (see again Figure 3). This conservative defect geometry is used here to obtain a preliminary estimate of the fuel temperature distribution (and temperature boundary values for the 3D model) and heater power. The fuel oxidation rate, the source term R_f^{react} in Eq. 1 and 5, is different in different azimuthal and radial locations in the 2D r - θ model. This can be shown if we plot the oxidation (or reduction) rate at the fuel-to-gas interface in the radial cracks at two azimuthal positions; just below the sheath defect at twelve o'clock (refer to Figure 5 (b)) and on the other side of the iridium wire at six o'clock, see the Figure 6.

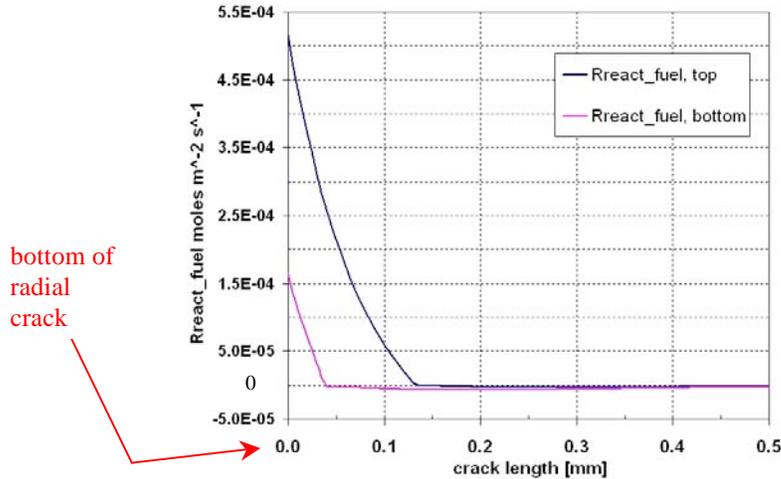


Figure 6: Fuel oxidation or reduction in radial cracks as a function of absolute radial position in the cracks from the r - θ model.

The source term R_f^{react} (or Rreact_fuel) can be positive (fuel oxidation) or can be negative (fuel reduction). This is determined by the local values of stoichiometric deviation X_{dev} in the fuel and the hydrogen molar fraction q of the gas in the cracks. As we can see from Figure 6, the oxidation rate far away from the defected sheath is much less than right under the defect site.

4.2 Oxidation of partial length 3D fuel element models

Solution of the fuel oxidation model in a 3D geometry represents a much more realistic solution than the 2D r - θ model analysis since the modelled defect size is specifically defined. Consider a line defect that is 1-mm wide and 5-mm long (a total defect area of 5-mm²); a defect geometry believed to be easily implemented in the out-reactor experiment. This type of defect has a 3D geometry as illustrated in Figure 2 and 7 (a). This model includes three radial cracks, which are 13 mm long in the axial direction. It is of note that a partial 10-cm length fuel element is modelled to reduce the computation time and memory requirements. The application of symmetry requires that only one quarter of the fuel element need to be modelled. This would also mean that the number of radial cracks actually modelled is five and the partial length of the model is actually 20-cm in length. The crack widths were increased to 25 μ m as opposed to the 15 μ m in the 2D r - θ model. In this model a pellet-pellet gap was included in the 3D model. It is conceivable that a gap may appear between two pellets under a sheath defect, allowing steam to more easily enter into this region. This gap is assumed to be present under the 1-mm wide by 5-mm long axial slit defect. The pellet-pellet gap was set 50 μ m in width, which was based on the axial gap in the fuel element [3] and consideration of pellet expansion due to thermal expansion only (model not shown here) of the out-reactor fuel pellets with dished end geometry at both pellet ends.

The 3D model does not include heat source terms, Zircaloy sheathing geometry, thermocouples or thermocouple holes. Instead boundary surface temperature values, indicated in Figure 7(a), which were derived from the r - θ model, were used. This was done to reduce the computational expense and solution time. Computer resources required were eight Xenon 2.67 MHz processors, 24-32 GB of RAM and ~10 hours processing time to solve partial length fuel elements.

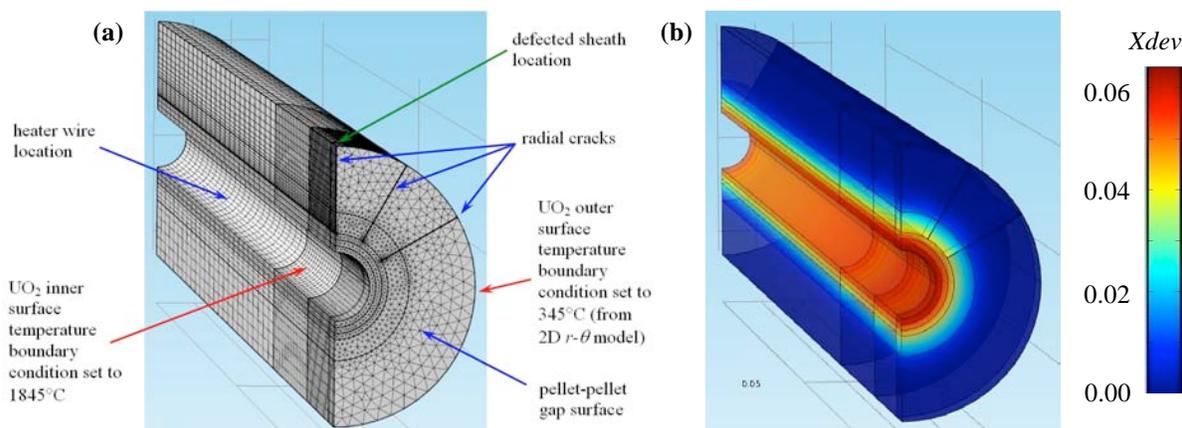


Figure 7: (a) Isometric view of 3D model with swept mesh, radial cracks, defected sheath location and temperature boundary conditions and (b) a distribution plot of oxygen stoichiometric deviation after 2 weeks of heating.

Figure 7 (b) gives the oxygen stoichiometric deviation result in the 3D model after two weeks of heating. Table 4 provides results for one and two weeks of heating for two cases. The first case is when oxidation occurs in the five radial cracks and surfaces in the pellet-pellet gap down to the crack depth (though not all surfaces were used).

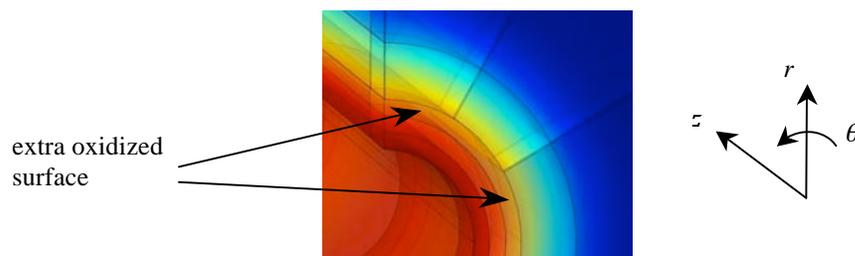


Figure 8: Close up view of the pellet-pellet gap model surfaces

The second case was the same as the first but with an extra surface in the pellet-pellet gap below the cracks (where it is hotter), see Figure 8. If the remaining surfaces below the cracks are modelled with the reaction term the maximum oxidation result could be higher than that stated in Table 3. Meshing sensitivity test will be done to confirm these preliminary results.

Table 3: Maximum oxygen stoichiometric deviation results for a 3D 20-cm long fuel element model with 1-mm by 5-mm slit defect under the defected sheath site.

3D model (20-cm long partial length fuel element)	Maximum X_{dev}	
	1 week of heating	2 weeks of heating
With surface area in the pellet-pellet gap up the crack tips depth	0.057	0.064
With increased surface area in the pellet-pellet gap below the crack tips	0.058	0.072

5. Conclusions

In this paper 2D r - θ and 3D fuel oxidation model simulations results were presented in support of a planned out-reactor fuel oxidation experiment. The 2D r - θ model was used to provide a close estimate of the temperature distribution in the fuel element cross section. The 3D model provided a more realistic result for predicting oxygen stoichiometric deviation in UO_2 fuel element because the defect size is specifically defined. A 1-mm wide by 5 mm long slit defect was investigated.

The inclusion of a pellet-pellet gap was investigated in the 3D model. The preliminary results show that if such a gap is present under a deliberate sheath defect an increased level of fuel oxidation may occur. Furthermore, if additional surfaces in the pellet-pellet gap (which are nearer to the iridium wire heater than are the radial cracks) are exposed to the steam environment, an additional increase in oxidation may result. The inclusion of the pellet-pellet gap under a defect in the 3D fuel oxidation model may prove to be useful in interpreting the out-reactor experimental results as well as in-reactor defective fuel performance.

Acknowledgements

The authors would like to acknowledge the useful feedback on finite element modelling provided by Farzin Abbasian at STERN Labs, Hamilton, Ontario.

References

- [1] J.D. Higgs, B.J. Lewis, W.T. Thompson and Z. He, "A conceptual model for the fuel oxidation of defective fuel", *Journal of Nuclear Materials*, 366 (2007) 99.
- [2] B.J. Lewis, F.C. Iglesias, D.S. Cox and E. Gheorghiu, "A model for fission gas release and fuel oxidation behaviour for defected UO_2 fuel elements", *Nuclear Technology*, 92 (1990) 353.
- [3] B.J. Lewis, R.D. MacDonald, N.V. Ivanoff and F.C. Iglesias, "Fuel performance and fission product release studies for defected fuel elements", *Nuclear Technology*, 103 (1992) 220.
- [4] D.R. Olander, "Oxidation of UO_2 by High-Pressure Steam", *Nuclear Technology*, 74 (1986) 215.
- [5] D.R. Olander, Y.S. Kim, W. Wang and S.K. Yagnik, "Steam oxidation of fuel in defective LWR rods", *Journal of Nuclear Materials*, 270 (1999) 11.
- [6] B.J. Lewis, B. Szpunar and F.C. Iglesias, "Fuel oxidation and thermal conductivity model for operating defective fuel rods", *Journal of Nuclear Materials*, 306 (2002) 30.
- [7] B.J. Lewis, W.T. Thompson, F. Akbari, D.M. Thompson, C. Thurgood and J. Higgs, "Thermodynamic and kinetic modelling of the fuel oxidation behaviour in operating defective fuel", *Journal of Nuclear Materials*, 328 (2004) 180.
- [8] H. Matzke, "Gas release mechanisms in UO_2 - A critical review", *Radiation Effects*, 53 (1980) 219.
- [9] W. Hüttig, H. Enker and M. Forberg, "In-Core surveillance of defective PWR fuel elements in the case of fuel-to-water contact", *Journal of Nuclear Materials*, 175 (1990) 147.
- [10] K. Une, M. Imamura, M. Amaya and Y. Korei, "Fuel oxidation and irradiation behaviours of defective BWR fuel rods", *Journal of Nuclear Materials*, 223 (1995) 40.

- [11] M. Limbäck, M. Dahlbäck, L. Hallstadius, P.M. Dalene, H. Devold, C. Vitanza, W. Wiesennack, H. Jenssen, B.C. Oberländer, I. Matsson and T. Andersson, “Test-reactor study of the phenomena involved in secondary fuel degradation”, Paper 1045, Proceedings of the 2004 International Meeting on LWR Fuel Performance, Orlando, Florida, 2004 September 19-22.
- [12] B. Cheng, B.C. Oberländer, W. Weisenack, S. Yagnik and J. Turnbull, “An in-reactor simulation test to evaluate root cause of secondary degradation of defective BWR fuel rod”, Zirconium in the nuclear industry: 13th International Symposium, ASTM STP 1423 (2002) 616.
- [13] A. Viktorov and M. Couture, Regulatory Activities in the Area of Fuel Safety and Performance, Fuelling A Clean Future, 9th International CNS Conference on CANDU Fuel, Location, 2005 September 18-21.
- [14] R.A. Verrall, Z. He and J. Mouris, “Characterization of Fuel Oxidation in Rods with Clad-Holes”, *Journal of Nuclear Materials*, 344 (2005) 240-245.
- [15] M. Oguma, “Cracking and relocation behaviour of nuclear fuel pellets during rise to power”, *Nuclear Engineering and Design*, 76 (1983) 35.
- [16] P.G. Lucuta, H. Matzke and R.A. Verrall, “Microscopic features of SIMFUEL - simulated high-burnup UO₂ based nuclear fuel”, *Journal of Nuclear Materials*, 178 (1991) 48.
- [17] J. Higgs, Modelling Oxidation Behaviour in Operating Defective Nuclear Reactor Fuel Element, Department of Chemistry and Chemical Engineering, Royal Military College of Canada, PhD Thesis, 2006.
- [18] Y. Sumi, L.M Keerand, and S. Nemat-Nasser, “Thermally induced radial cracking in fuel element pellets”, *Journal of Nuclear Materials* 96 (1981) 147.
- [19] C. Bernaudat, “Mechanical behaviour modelling of fractured nuclear fuel pellets”, *Nuclear Engineering and Design*, 156 (1995) 373.
- [20] D.R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, University of California, Technical Information Center, Energy Research and Development Administration, 1976, US Department of Energy, Prepared for Publishing by HP, reprint from the University of Michigan Libraries Collection.
- [21] Nuclear Engineering International, September 2010, www.neimagazine.com.
- [22] M.J.F. Notely, ELESIM: A computer code for predicting the performance of nuclear fuel elements, *Nuclear Technology* 44 (1979) 445.
- [23] K. Shaheen, A.D. Quastel, J.S. Bell, B.J. Lewis, W.T. Thompson and E.C. Corcoran, Modelling CABDU fuel element and bundle behaviour for in-reactor and out-reactor performance of intact and defective fuel, 11th International Conference on CANDU Fuel, Niagara Falls Ontario, Canada, 2010 October 17-20.
- [24] J.C. Bailar, Jr. Therald Moeller, Jacob Kleinberg, Cyrus O. Guss, Mary E. Castellion and Clyde Metz, Chemistry, Academic Press, 1989
- [25] W.B.J. Zimmerman, Multiphysics Modelling with Finite Element Methods, World Scientific Publishing Co. Pte. Ltd., London, 2006.
- [26] COMSOL Multiphysics Version 3.5a and Version 4.1 finite element modelling and simulation commercial software, www.comsol.com.
- [27] R.E. Williford, A cracked-fuel constitutive equation, *Nuclear Technology* 67 (1984) 208.