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Development and testing of the FAST fuel performance code: Transient conditions (Part 2)



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HIGHLIGHTS

- FAST is a general purpose nuclear fuel model for both normal and transient conditions.
- Multiphysics, multi-dimensional approach using COMSOL multiphysics.
- Present the extension of the code for high temperature transient conditions and multi-pellet geometries.
- Compares code predictions to experimental data of simulated loss of coolant accident.
- Demonstrates good agreement with temperature and sheath strain measurements.

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ABSTRACT

This paper documents the extension of the Fuel And Sheath modeling Tool (FAST) for modeling transient conditions and presents a proof of concept validation exercise. This validation compares the predictions of FAST and ELESTRES/ELOCA fuel performance codes against experimental measurements from a simulated loss of coolant test conducted at Chalk River Laboratories. The comparison includes in reactor measurements of fuel temperature and internal gas pressure along with post irradiation (hot-cell) measurements of cladding deformation and oxidation. The results of this comparison show that the single pellet version of the FAST code was insufficient to fully account for strong axial dependence along an element. This was addressed by modifying the FAST code geometry to allow an arbitrary number of pellets in the fuel-stack. This full element version demonstrated improved agreement with measured cladding deformation, including circumferential ridging effects.

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1. Introduction

Historically, separate fuel modeling codes were developed for simulating fuel under normal operating conditions (NOC) and high-temperature transient (accident) conditions. This division allowed each code to include a different subset of physics important for different temperatures and timescales. The application of FAST for NOC was published as Part I (Prudil et al., n.d.). This paper is Part II, which describes the use of FAST for transient applications.

Codes for NOC focused on modeling the behavior of the fuel over the time-span of days to years. At these timescales, behavior is expected to be dominated primarily by changes in fuel burnup, densification and swelling, fission gas release, and sheath creepdown. Transient fuel modeling codes generally required modeling fuel at high temperatures but for much shorter periods of time, typically seconds to minutes. In this domain, behavior is expected to be dominated by rapid changes in linear power, temperature, gas pressure and coolant conditions. The higher temperatures can also lead to additional effects such as phase changes, sheath ballooning and sheath oxidation. This fuel modeling paradigm has been employed for the LWR fuel modeling codes GAPCON+FRAP-T (Hann et al., 1973; Thompson et al., 1975) and FRAPCON+FRAPTRAN (Gelhood et al., 2011) as well as the CANDU ELESTRES+ELOCA (Hallgrimson et al., 1992; Tayal, 1987) codes (previously ELESIM+ELOCA).

In addition to the differences in physics, the numerical methods of solution can also differ between NOC and transient codes.

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Typically NOC codes have used implicit time-integration schemes because they are stable with large time-steps, even though each step is more computationally expensive. However, transient fuel modeling codes model fuel over a comparatively short period of time enabling them to use explicit time stepping. Explicit time-stepping is particularly advantageous for highly non-linear problems requiring many short time-steps.

Despite the separation of the physics into two codes, the behavior of the fuel varies continuously between the low-temperature long time scales regime and high-temperature short time scales regime. It is therefore desirable to develop fuel models which are able to simultaneously model long- and short-timescale phenomena over a wide range of temperatures, effectively unifying the steady-state and transient fuel models into one self-consistent model. This has already been achieved by a number of advanced LWR fuel performance codes such as FALCON (Electric Power Research Institute (EPRI), 2004), TRANSURANUS (Lassmann, 1992; Lassmann et al., 1998), FEMAXI (Nuclear Energy Agency, 2011), and BISON (Williamson et al., 2012; Hales et al., 2014).

In this work, we extended the FAST code for NOC to include the capability for modeling high-temperature fuel transients; making the FAST code the first unified model for CANDU fuel. The transient application requires the addition of high-temperature creep phenomena, sheath oxidation, and time-dependent irradiation conditions.

One feature of the unified code architecture is that both high and low temperature phenomena are available for all cases as dictated by the instantaneous state of the fuel (instead of being limited to only high or low temperature phenomena). The physics models determine the rate (kinetics) of each phenomena according to the current conditions. For example, the growth rate of the oxide layer is determined by the sheath surface temperature and current oxide thickness. At low temperatures the model predicts a near zero oxidation rate (equivalent to the oxidation model disabled), while at higher temperatures the oxidation rate may become substantial. Users need only specify the element details (such as geometry, grain size, enrichment, fill gas), the initial conditions (such as temperature, oxide thickness) as well as the irradiation conditions (such as linear power history and coolant conditions, which may be functions of time, burnup or other dependent variables). In order to support modeling both short and long time-scale phenomena FAST code utilizes the built in variable step size backwards difference formulation (BDF) available in COMSOL (COMSOL AB, 2014). This is based on the Implicit Differential-Algebraic (IDA) from the SUNDI-ALS package (Hindmarsh et al., 2012).

2. Model development

In Part 1, only the models relevant for simulating fuel under NOC were discussed. At higher temperatures these models are still active; however, there are additional phenomena which need to be accounted for. In this section, the models for these additional phenomena are presented along with the modeling theory utilized by FAST.

2.1. High temperature sheath creep

In the FAST code, cladding creep phenomena was divided into low- and high-temperature domains. The creep in the low temperature domain, defined as below 700 K, consisted of thermal and irradiation creep (as described in Part 1). Above 700 K, these terms are replaced with the NIRVANA high-temperature creep model developed by Sills and Holt of AECL (Sills and Holt, 1979). The model has been validated for temperatures from 700 K to 1600 K with creep strain rates ranging from $10^{-5} \, \text{s}^{-1}$ to $10^{-1} \, \text{s}^{-1}$.

The NIRVANA creep rate model is a function of the equivalent stress, σ_{eqv} (Pa), which is a measure of the total stress at a point due to combined loads in different directions. It is given by:

$$\sigma_{\text{eqv}} = \sqrt{F_{\text{Hill}}(\sigma_{\theta} - \sigma_{z})^{2} + G_{\text{Hill}}(\sigma_{z} - \sigma_{r})^{2} + H_{\text{Hill}}(\sigma_{r} - \sigma_{\theta})^{2}}$$
(1)

where $\sigma_{\rm r} \, \sigma_{\rm \theta}$ and $\sigma_{\rm z}$ are the stress in the radial, circumferential and axial directions, respectively. The coefficients $F_{\rm Hill}$, $G_{\rm Hill}$ and $H_{\rm Hill}$ are the Hill anisotropy parameters of the material which account for crystallographic texture. The FAST code utilizes, the Hill parameters for as-fabricated CANDU fuel sheathing, which are $F_{\rm Hill}$ = 0.773, $G_{\rm Hill}$ = 0.532 and $H_{\rm Hill}$ = 0.195. If the microstructure is significantly altered by high-temperatures or large plastic strains the value of these parameters will change. However, this dependence is not considered in the FAST code.

The expression for the creep rate due to grain-boundary sliding in units of s^{-1} is given by:

$$\frac{d\varepsilon_{\rm gb}}{dt} = 6.34 \times 10^{-6} \left(\frac{\sigma_{\rm eqv}}{Gg_{\rm d}}\right)^2 \exp\left(\frac{-9431}{T}\right) \tag{2}$$

where, G is the shear modulus of the sheath in Pa, g_d is the average grain diameter in m and T is the temperature in K. This type of creep occurs when the boundaries between crystals, which are weakly bonded, slide past each other due to the applied load.

Dislocation creep (or dislocation glide) occurs when crystal-lographic dislocations move. The dislocations act as obstacles to plane-of-atoms sliding past each other. When the dislocations move out of the way, a slip plane can form, resulting in dislocation creep. This is modeled using the internal-stress field, $\sigma_{\rm int}$ (T), which represents the retarding effect of crystallographic dislocations on the creep. This leads to an effective stress, $\sigma_{\rm eff}$, which is given by:

$$\sigma_{\text{eff}} = \max(\sigma_{\text{eqv}} - \sigma_{\text{int}}(T), 0) \tag{3}$$

The magnitude of the retarding effect is dependent on density of the dislocations and their mobility which is temperature dependent. To account for this, the internal stress in the ELOCA code is scaled according to:

$$\sigma_{\rm int}(T) = \sigma_{\rm int}(T_0) \frac{E(T)}{E(298 \,\mathrm{K})} \tag{4}$$

where E is the Young's Modulus of Zircaloy-4 as a function of temperature. It should be noted that this scaling is not documented in the open literature of the NIRVANA model. It is known to be used when the ELOCA code utilizes the ELESTRES results at the start of a transient (using T=700 K). For the FAST code this scaling is continuously applied, although this may not be identical to the implementation in NIRVANA or ELOCA.

The dislocation creep strain, ε_d (unitless), and the internal stress, in units of Pa, are found by solving the following coupled ODEs on the sheath domain:

$$\frac{d\varepsilon_{\rm d}}{dt} = 2.98 \times 10^{-28} \exp\left(\frac{-34726}{T}\right) \sigma_{\rm eff}^{5.3} \tag{5}$$

$$\frac{d\sigma_{\text{int}}(T_0)}{dt} = 4.767 \times 10^{-30} E(T_0) \exp\left(\frac{-34726}{T}\right) \left(\sigma_{\text{eff}}^{5.3} - \frac{\sigma_{\text{int}}\sigma_{\text{eff}}^{4.3}}{0.33}\right) - A_{\text{int}} + B_{\text{int}}$$
(6)

The initial value of the internal stress is dependent on the manufacturing process. For CANDU fuel, an initial value of $53.4 \,\mathrm{MPa}$ is used. The variable A_{int} represents rate of dislocation healing by recrystallization and B_{int} is the rate of production by low temperature plastic deformation (cold work) and from radiation. The

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