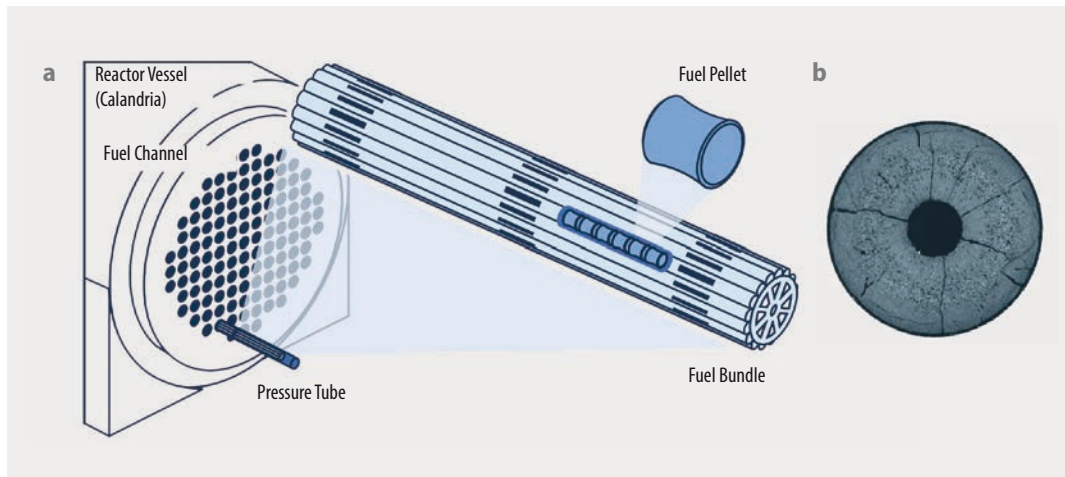# Complex Material Behavior Illuminated

At Canadian Nuclear Laboratories, multiphysics simulation is used to shed light on the complex material behavior of nuclear fuel.

Andrew Prudil

Fig. 1 In a nuclear reactor, pristine nuclear fuel pellets are placed inside the cladding, or sealed metal tube (a). A transverse micrograph of a fuel pellet shows the microstructure produced during operation (b).

What happens when engineers explore the possibility of replacing tried-and-true but cumbersome in-house code with multiphysics simulation software? Nuclear engineers began to ask this question at the Computational Techniques Branch of Canadian Nuclear Laboratories (CNL), Canada's premier nuclear science and technology organization.

In the field of nuclear engineering, where research focuses on improving the safety, efficiency, and economics of reactors, mature and robust in-house computer codes are frequently used for modeling studies. Unfortunately, the need to comb through many lines of code to investigate the potential effect of a minor adjustment to a system is a real barrier to innovation.

As an alternative to modifying mature or legacy codes, a multiphysics platform provides an environment that allows engineers to explore changes in data and modeling methods without the complications of adapting lengthy code.

Simulation software helps to find ways to improve the established, seemingly immutable design of nuclear reactors. Nuclear science is material science, but with additional considerations for the effects of radiation. The materials include the nuclear fuel, as well as the constituents of some of the surrounding components.

The Complexity of Nuclear Fuel

Multiphysics software is used to create an awe-inspiring mathematical model that includes a staggering number of physical phenomena. The modeling work includes a representation of a nuclear fuel pellet including heat transport, structural mechanics deformation, mechanical contact, pressure buildup due to fission gas release, and microstructural changes due to grain growth, radiation damage, and burnup. It is also possible to model the behavior of the cladding around the nuclear fuel.

In a nuclear reactor, pristine nuclear fuel pellets are placed inside the cladding, or sealed metal tube (**Fig. 1**). Upon irradiation, these fuel pellets
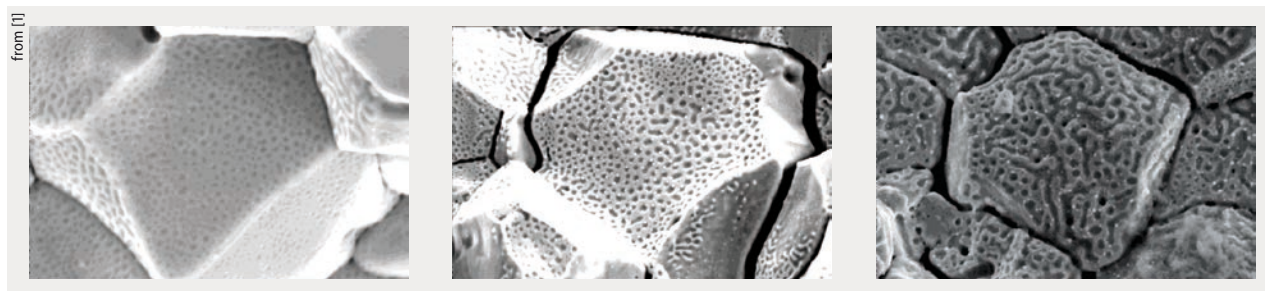

Fig. 2 These micrographs show the development of fission gas bubbles on the grain boundaries of uranium dioxide fuel. With increasing burnup, left to right, the bubbles become larger and more interconnected. White, Development of grain-face porosity in irradiated fuel.

increase in temperature, and transfer heat to the sealed metal tube, which in turn transfers heat to water. This hot water is eventually used to produce steam in order to generate electricity, mirroring the process that takes place in conventional power plants.

Upon irradiation, a fission reaction drives heat production within the fuel pellets, resulting in high temperatures, high thermal gradients, and thermal expansion. There are also nuclear-specific phenomena to consider, as the products of fission accumulate in the fuel pellets.

Fig. 1 shows the complicated micro-structure of a nuclear fuel pellet after sustained high-temperature opera-tion. The initial as-fabricated grain structure remains only on the out-side closest to the coolant where the temperature is the lowest. At slightly higher temperatures, the grains grow (coarsen), forming a region of equi-axed grain growth. At the highest tem-peratures, a vapor transport mecha-nism enables the porosity in the fuel to migrate following the temperature gradient (toward the center) forming a central void and leaving long colum-nar grains in its wake.

Of these effects, cracking occurs inside the ceramic fuel. There is also contact between the ceramic and the metal cladding. Radiation damage needs to be considered, as high energy fission products such as gamma and neutron radiation change the micro-structure of all materials. There is also macroscopic swelling, as fission is the splitting of one atom into two, and two atoms take more space than one. Fur-thermore, two fission products, the
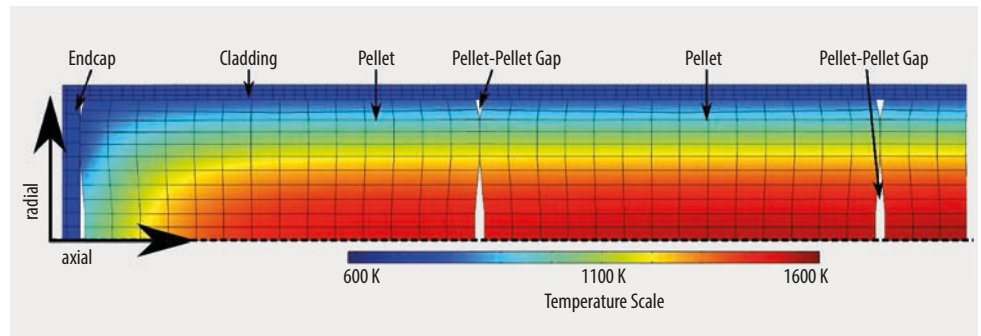
Fig. 3 Simulation results from the Fuel and Sheath Modeling Tool (FAST) show the temperature throughout the cladding, fuel pellets, and pellet-pellet gaps.

noble gases xenon and krypton, are inert and form bubbles inside the fuel pellets (**Fig. 2**).

There are also corrosion issues to consider as high-temperature water in a radiation environment leads to the formation of radiolysis products, which cause corrosion on the outside of the cladding.

Preventing Fuel Failure

Because the properties of nuclear fuel pellets change dramatically as they are irradiated, engineers rely heavily on models to predict fuel performance parameters like peak temperature, gas pressure, and cladding strain to inter-polate between available experiments. Similarly, knowing how any design change could manifest in a radiation environment requires extensive mo-deling work and validation with phy-sical measurements.

One of the primary motivations for this research was to model the defor-mation of the cladding and obtain a better estimate of cladding strain, as it is a significant mechanism of fuel

failure. Once a model for strain of the cladding was created, the system could be optimized virtually. Opti-mization strategies include making a direct change to the fuel, the fuel to cladding gap, or how the fuel is treated once in the reactor.

It's relatively straightforward to build a model, but less straightforward to know what the correct material pro-perties are to put in that model, espe-cially when they evolve with time and radiation exposure. After completing a new model, the simulation results are compared to experimental results to assess the quality of the predictions.

Changing the fuel itself is an attrac-tive approach to improving a nuclear reactor, as nuclear fuel is designed to be replaced. This is cost effective, as no parts of the reactor would need to be updated: The engineers could sim-ply feed the system the new fuel when it is time to refuel the reactor.
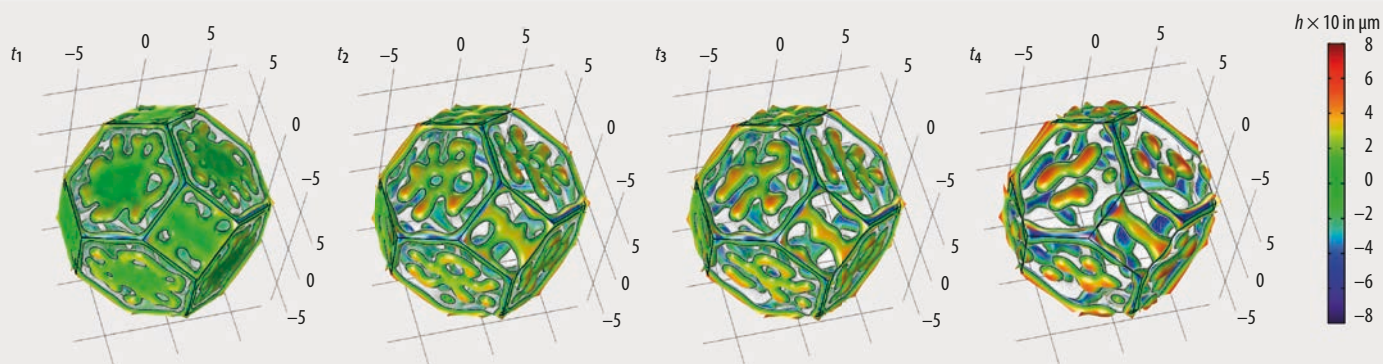
One Model for Many Phenomena

Using the COMSOL Multiphysics® software, the Fuel and Sheath Mode-
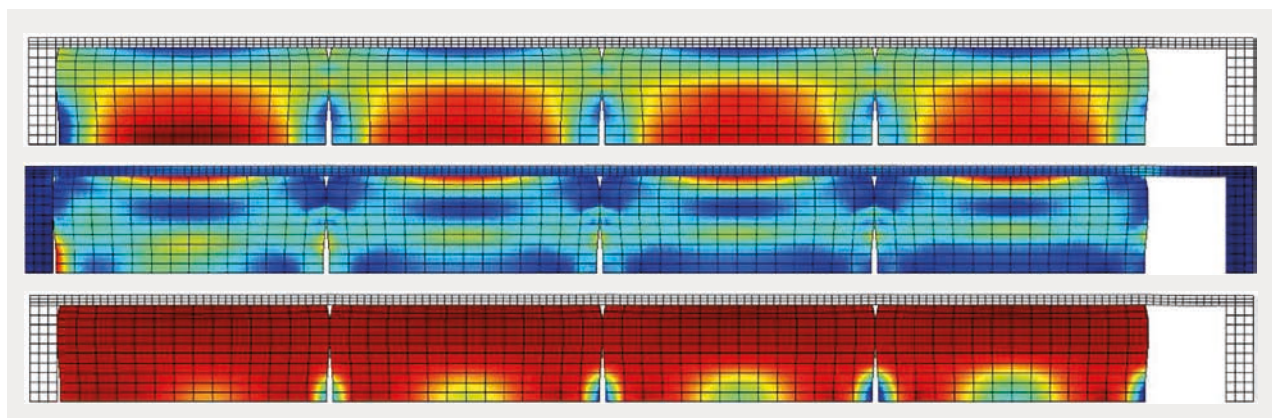
Fig. 4 Simulation results from FAST show hydrostatic pressure (top), von Mises stress (middle), and axial creep (bottom) throughout the cladding, fuel pellets, and pellet-pellet gaps.

Fig. 5 The simulation (left to right) shows formation, movement, and coalescence of gas bubbles on the grain boundaries.

ling Tool (FAST) was created to capture the complex heat transport, solid mechanics, and material behavior of the nuclear fuel, cladding, and the gap between the fuel and the cladding. **Fig. 3** shows an example of the temperature profile generated for the pellets and cladding.

Using COMSOL software, one doesn't have to worry much about the numerics and programming. The software allows to directly approach the math and the physics rather than worry about the solution process and the post-processing.

Simulation results from FAST also show hydrostatic pressure, von Mises stress, and axial creep throughout the cladding and fuel pellets (**Fig. 4**). The distribution of these fields is the result of design parameters such as the length-to-diameter ratio and chamber dimensions as well as operational considerations like power level and coolant temperature.

Grain Boundary Porosity Simulated

To extend the modeling tool and shed light on the performance of the reac-

tor in a different way, the diffusion of gas out of the fuel grains was modeled, and then the formation and movement of bubbles on the grain boundaries (**Fig. 5**) using the equation-based modeling functionality available in COMSOL®.

Upon irradiation and the chemical change of the nuclear fuel, gas seeps out of the fuel grain, forming bubbles. These bubbles then move around and coalesce (**Fig. 5**). In a traditional phase field, the volume of the fuel grains would be modeled. The novelty and power of this technique comes from ignoring the solids and only modeling the moving surface between the solids and gas. This turns a 3D problem into 2D and significantly reduces the computational resources required.

The model uses two coupled weak form equations on the surface of the grain, one for the distance to the bubble surface, and the other for the chemical potential. Knowing how much gas comes out of the fuel allows to calculate the thermal conductivity and gas pressure inside the fuel element. The results from this analysis help to determine other key indicators of fuel performance. This set of calculations serves as a nonlinear representation of fuel degradation (**Fig. 6**).

From the simulation, it is possible to approximate if the pressure is

sufficiently low, such that the fuel can continue being irradiated – an insight with great implications for safety.
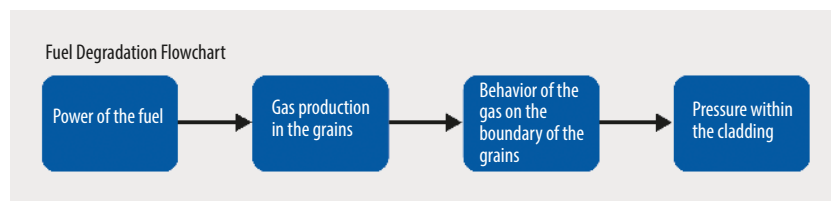
Simulation Drives Innovation

By using multiphysics simulation, engineers at CNL were able to create a useful tool and clear the way for faster design iteration and innovation. In addition, multiphysics simulation can influence other areas of development in nuclear engineering, such as the development of accident-tolerant fuel. The interest in designing fuel that is resistant to severe accident scenarios represents an opportunity for engineers to completely rethink fuel.

In the long term, simulation software can play a role in the development of small module reactors, which would represent a paradigm shift in nuclear reactor design toward smaller, easier to build reactors and potentially reduce the high capital costs of reactors. Small module reactors could be made of new materials and have new geometries and safety paradigms, a departure from the decades-long trend of ever-larger nuclear reactors.

Meanwhile, the complex representation of existing reactors continues to lend valuable insight into the many layers of complexity of the nuclear reactor.

[1] *R. J. White*. Nuc. Mat. **325**, 61 (2004), www.sciencedirect.com/science/article/pii/S0022311503004616

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Fuel Degradation Flowchart

Power of the fuel → Gas production in the grains → Behavior of the gas on the boundary of the grains → Pressure within the cladding

Fig. 6 The set of calculations that determines key indicators of fuel performance serves as a nonlinear representation of fuel degradation.