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CAMPUS: A FULLY COUPLED MULTIPHYSICS MODELING APPROACH FOR LIGHT WATER FUEL PERFORMANCE

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ABSTRACT – Light water fuels operate in an environment that involves complex multiphysics phenomena, and the multiphysics behavior is often tightly coupled. A fuel performance code called CityU Advanced Multiphysics Nuclear Fuels Performance with User-defined Simulations (CAMPUS) was developed to predict light water reactor fuel behavior. CAMPUS code considers heat generation and conduction, oxygen diffusion, thermal expansion, elastic strain, densification, and fission product swelling, grain growth, fission gas production and release, gap heat transfer, mechanical contact, gap/plenum pressure with plenum volume, fuel thermal and irradiation creep, cladding thermal and irradiation creep and oxidation. All the equations are implemented into COMSOL Multiphysics finite-element platform with a 2D axisymmetric geometry of a fuel pellet with cladding. Comparisons of critical fuel performance parameters for UO_2 fuel using CAMPUS are similar to those obtained from BISON, ABAQUS and FRAPCON. The capabilities of the CAMPUS code were further demonstrated by simulating the performance of oxide fuel (UO_2), mixed oxide fuel ($(Th_{0.9},U_{0.1})O_2$), and accident tolerant fuels, for example, enhanced thermal conductivity UO_2-BeO, UO_2-SiC and U_3Si_2 fuels, under normal operation conditions. These demonstrate that CAMPUS is a practical tool not only for the existing LWR fuel performance modeling but also for new fuel design, development and behavior prediction.

Introduction

Nuclear fuels operate in an environment that involves complex multiphysics phenomena, and the multiphysics behavior is often tightly coupled. The prediction of fuel behavior under irradiation involves very complex material behavior that is not seen in any other engineering discipline. Understanding and predicting the evolving material properties and phenomenal behaviors of nuclear fuels are major challenges for fuel design and behavior prediction. The multiphysics behavior is often a tightly coupled thermal, mechanical and chemical phenomenon associated with a large number of control parameters and uncertainties, which requires an advanced fuel performance modeling and simulation capability to improve the existing reactors performance, to address environmental and reactor safety concerns. Nuclear fuel performance modeling and simulation capability is necessary as a result of the high cost and difficulty in experimental measurements. So, a fuel performance code called CityU Advanced Multiphysics Nuclear Fuels Performance with

User-defined Simulations (CAMPUS) was developed to predict both light water reactor fuel behavior.

1. Previous Approaches

Early fuel modelling codes employed a fixed one-dimensional or quasi-two-dimensional representation of the fuel geometry such as GAPCON [1], FALCON [2], FEMAXI [3], FRAPCON [4] and FRAPTRAN [5]. These codes typically utilized many empirical correlations with limited coupling between phenomena. Some notable French codes (TOUTATIS [6] and ALCYONE [7]) employed three-dimensional geometries and are used to investigate localized behavior (such as pellet cracking or pellet cladding interactions). However, in general, fuel modeling codes have usually been written as standalone computer programs. The disadvantage of this approach is that such codes are typically restrictive for the end user since much of the functionality is hard-coded. This implies a significant modification (editing) to the source code is required for a different application.

The BISON code [8] from Idaho National Laboratory (INL) employed a full set of multidimensional multiphysics capabilities. The code is highly scalable and applicable to solving 1D, 2D axisymmetric and 3D nuclear fuel performance problems [9]. This is accomplished by making use of the numerical solution capabilities of the Multiphysics Object Oriented Simulation Environment (MOOSE) framework (also developed at INL), which is a general purpose, free and open source numerical simulation tool applicable far beyond the nuclear industry (note that BISON is also open source, however, it is export controlled and must be obtained from INL). The MOOSE platform was also adapted for the HORSE code for modeling the thermomechanical behavior of CANDU Fuel in 3D [10]. The MOOSE framework includes a limited graphical user interface and lacks some pre-and-post-processing tools (these tasks are usually performed using additional 3rd party software packages such as Cubit/Trelis, Gmsh). Similarly, Williamson [11] used ABAQUS, another well-known multipurpose finite-element tool, to enhance the modeling of LWR fuel rods with multi-pellets under steady-state and transient conditions. The BISON code is not an open source and also needs a long time to develop, and one has to have intimate knowledge of the internal structure of the code for modeling different fuels and/or geometries.

The FAST code was developed using COMSOL Multiphysics software to simulate the CANDU reactor fuel performance under normal and transient conditions [12 and 13]. The FAST code assumes azimuthal symmetry allowing the use of a 2 dimensional (radial-axial) representation of the fuel element geometry including pellet dishing, chamfering and central holes. It can directly model complete stacks of pellets (and accompanying cladding) or it can also assume that the single pellet is representative of all pellets within an element (using a periodic boundary condition in the axial direction). The code is intended for use for both normal and transient conditions and includes models for temperature, displacement, grain size, burnup, densification, swelling, fission gas diffusion and release to grain boundary, pellet-to-pellet gap size, pellet-to-sheath gap size and sheath creep. It has undergone proof-of-concept validation against experimental data and comparison with the ELESIM [14], ELESTRES [15] and ELOCA [16] codes used for CANDU fuel. The FAST code is used primarily for modeling PHWR fuel performance.

2. CAMPUS Code Structure

In this paper, the development of a new code called CityU Advanced Multiphysics Nuclear Fuels Performance with User-defined Simulations code (CAMPUS) is described, which has been using the COMSOL Multiphysics platform. This is a flexible commercial finite-element platform that solves a wide range of ordinary and partial differential equations (ODEs and PDEs) with arbitrary coupling of the dependent variables. The CAMPUS code is intended for use in education, research and design applications within the LWR community such as design of fuel experiments, evaluations of fuel concepts, and assessment of models. We adopted the modeling methodology from the FAST code [17] by modifying the fuel geometry and the detailed physical models to model LWR reactor fuel performance. The authors have integrated LWR fuel performance models from MATPRO [18], BISON [9], and FAST code [17] into CAMPUS.

The CAMPUS code considers heat generation and conduction, constituent diffusion, thermal expansion, elastic strain, densification, and fission product swelling, grain growth, fission gas production and release, gap heat transfer, mechanical contact, gap/plenum pressure with plenum volume, fuel thermal and irradiation creep, cladding thermal and irradiation creep and oxidation. The multiple physics are considered for all the components of fuel, cladding, gap and coolant of fuel assembly as well as power generation, neutron flux and fuel burnpup, and all the physics are interrelated as described in Figure 1.

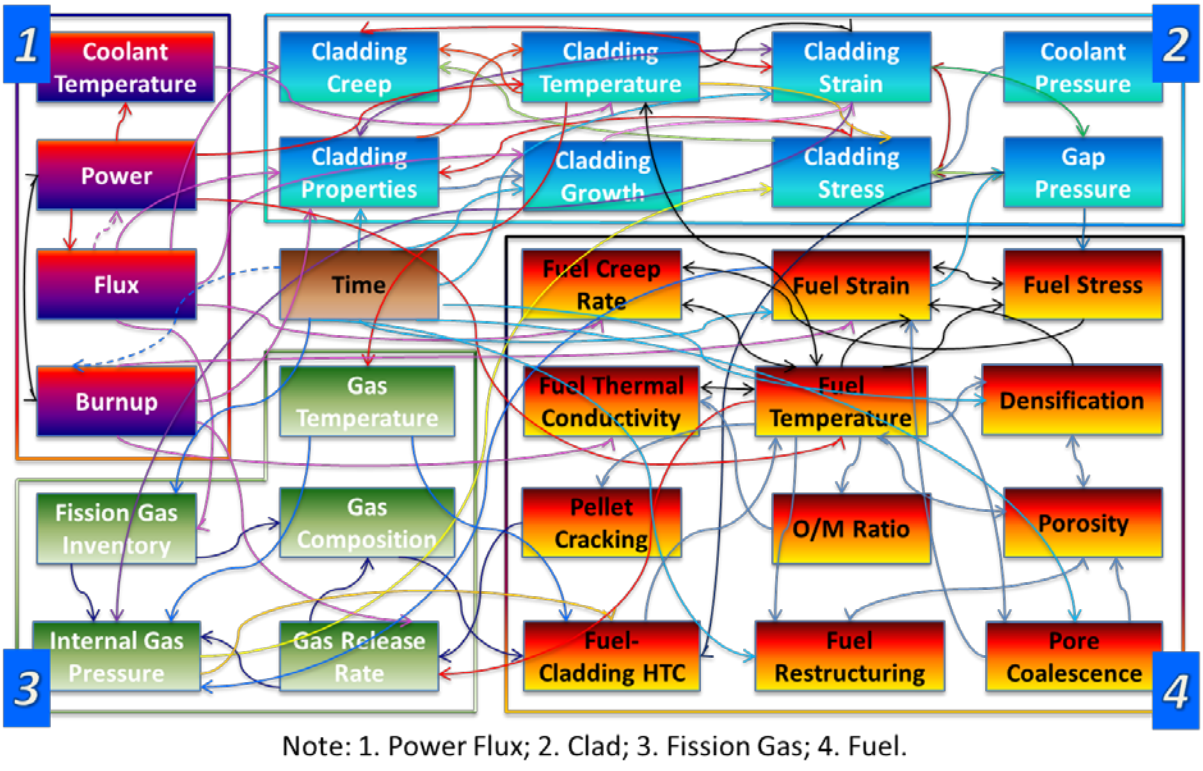


Figure 1 Multiphysics and multiscale nuclear fuels performance

The modeling and simulation code structure of CAMPUS [19] is shown in Figure 2. All the equations are implemented into COMSOL Multiphysics finite-element platform with 2D axisymmetric or 3D geometries of a fuel pellet with cladding. Multiple time and length scales are adopted for multi-physics phenomena fully coupled under irradiation of light water reactors. The details about the implementation of behavioral models and material properties can be found in [20].

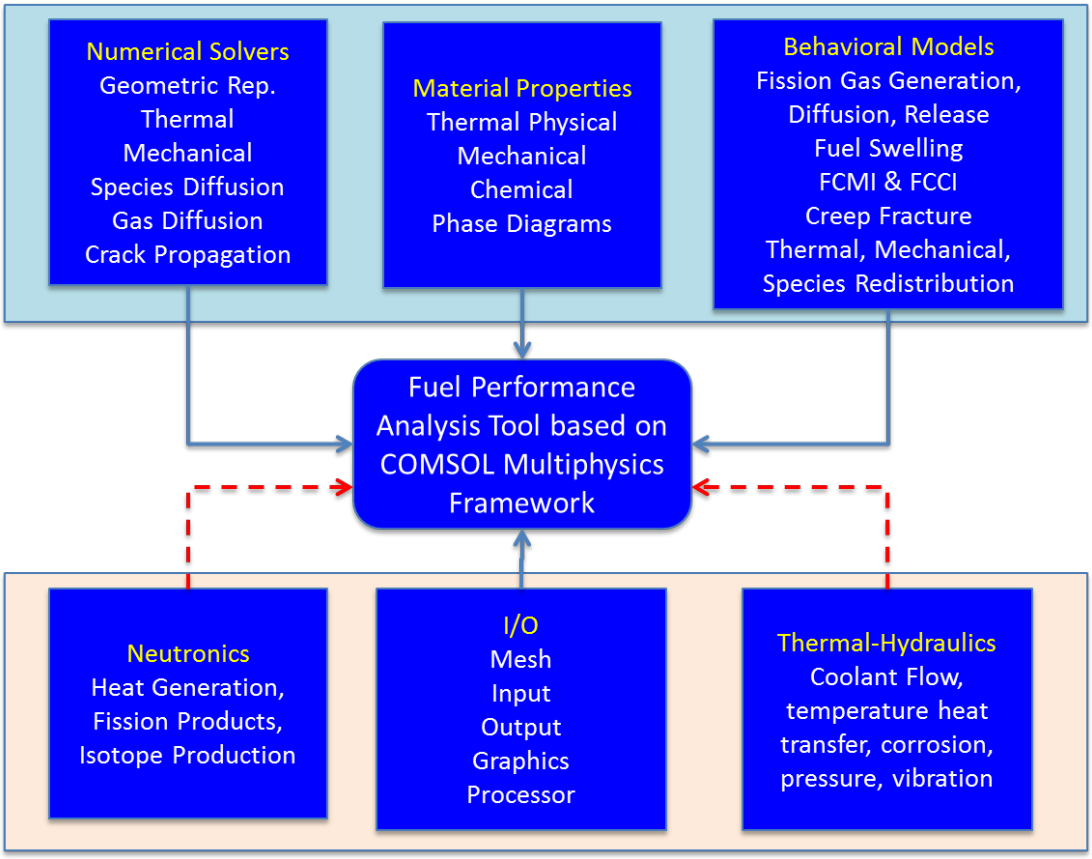


Figure 2 CAMPUS nuclear fuel performance modeling and simulation code structure. [19]

3. CAMPUS Verification and Validation

To verify and validate the CAMPUS code simulation capability, a comparison of the CAMPUS code predictions was performed for UO_2 fuel behavior in a light water reactor against those from BISON [8], ABAQUS [11] and FRAPCON codes. Figure 3 shows the predicted temperatures at the fuel centerline, fuel outer surface and cladding inner surface during power up and steady state operation with four codes. Figure 4 shows the gap closure vs. fuel burnup. The gap is found to be closed at a burnup of about 35 MWd/kg-U by the CAMPUS prediction, while the values from BISON and ABAQUS are about 34 MWd/kg-U and 32 MWd/kg-U, respectively. The gap size from FRAPCON is found to decrease dramatically (which can be ascribed to the different mechanical model used) and reach 1.5 microns (~approximately the surface roughness) at 32 MWd/kg-U till the end of the simulation, indicating an earlier gap closure. Figure 5 shows the fission gas release and plenum pressure evolutions vs the fuel burnup. The fission gas release from CAMPUS was earlier than from BISON, and the release fraction was a little bit

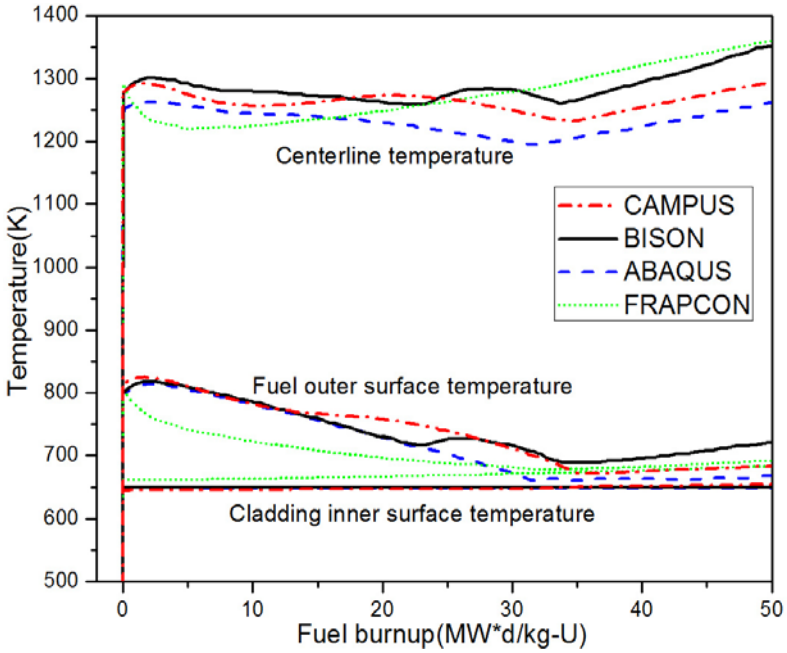


Figure 3 Temperature profile comparisons of four codes. The red dash with dotted line is from CAMPUS, black solid line from BISON, blue dash line from ABAQUS, and green dotted line from FRAPCON. [20]

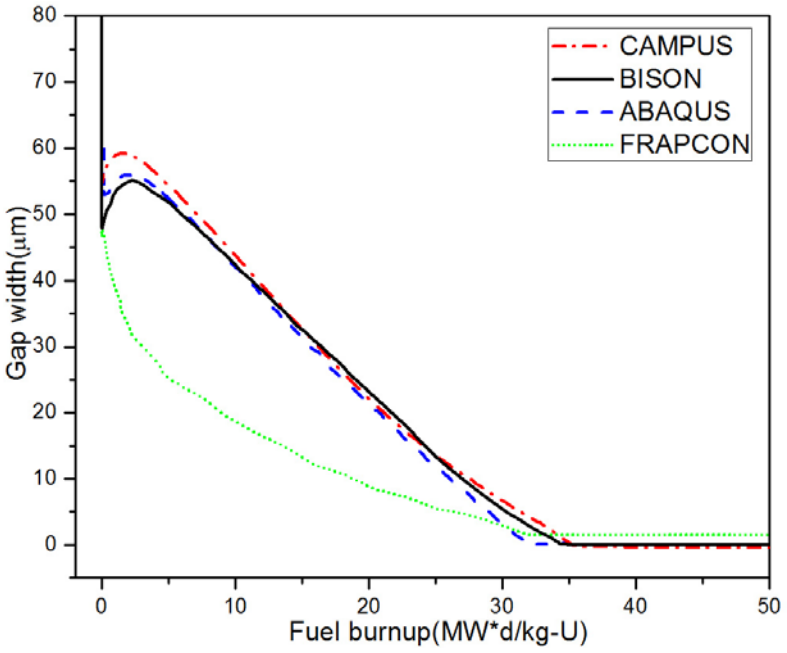


Figure 4 Gap size comparisons of four codes. The red dash with dotted line is from CAMPUS, black solid line from BISON, blue dash line from ABAQUS, and green dotted line from FRAPCON. [20]

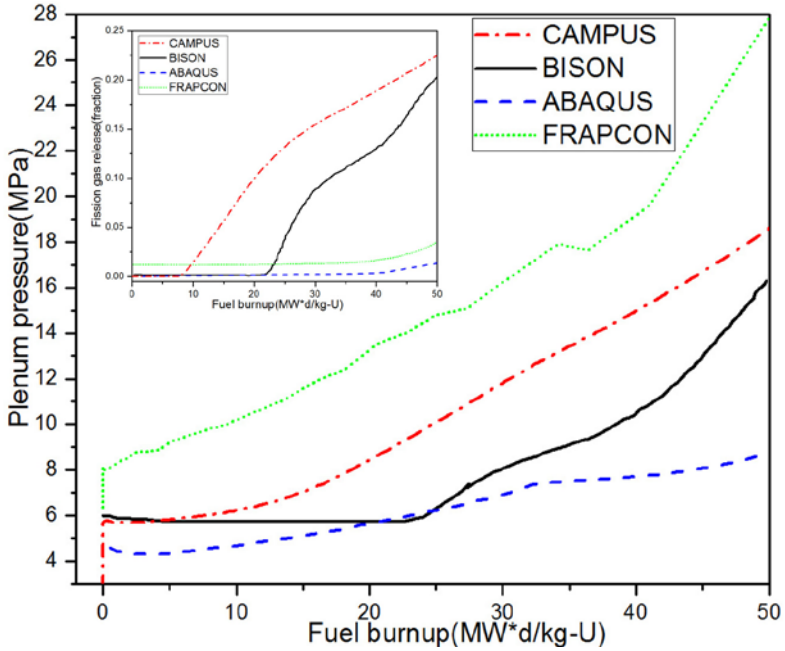


Figure 5 Plenum pressure comparisons of four codes. Inset shows the comparisons of fission gas release. The red dash with dotted line is from CAMPUS, black solid line from BISON, blue dash line from ABAQUS, and green dotted line from FRAPCON. [20]

larger than BISON, which further induced a higher plenum pressure, pushing the cladding outward and delaying gap closure. The fission gas from ABAQUS and FRAPCON started to release at a very high burnup level and released only a small fraction. This could be ascribed to different fission gas release model used compared to BISON and CAMPUS. In general, the CAMPUS predictions are found to be consistent with those from the other codes. Some differences among the code predictions attribute to the models employed, for example, fuel densification and fission gas release models.

4. CAMPUS Capability Demonstration

The advanced fuel modeling capability of CAMPUS was demonstrated by performing analysis for different fuel types, including oxide (UO_2) (as a baseline), composite (UO_2-10%volBeO), silicide (U_3Si_2), mixed oxide ($(Th_{0.9},U_{0.1})O_2$). The temperature profile, as shown in Figure 6(a), shows that the UO_2 fuel achieves the highest centerline temperature, while the U_3Si_2 fuel has the lowest fuel centerline temperature. Figure 6 (b) shows the gap size evolution of these four cases. The U_3Si_2 fuel experiences the fastest gap closure, which is caused by the large thermal expansion coefficient. Compared to the gap closure time of UO_2, the UO_2-10vol%BeO fuel tends to delay the gap closure time, which can help to minimize fuel and cladding mechanical interaction. Unexpectedly, the gap closure time for $(Th_{0.9},U_{0.1})O_2$ fuel was found to be earlier than UO_2 despite undergoing less thermal expansion. This was a result of the lower internal pressure due to the lower fission gas release enabling faster creep down of the cladding.

Figure 7(a) shows the $(Th_{0.9},U_{0.1})O_2$ fuel has the lowest plenum pressure and fission gas release fraction, as the fission gas diffusion coefficient is approximately 10% of the value for UO_2 and the fuel temperature of

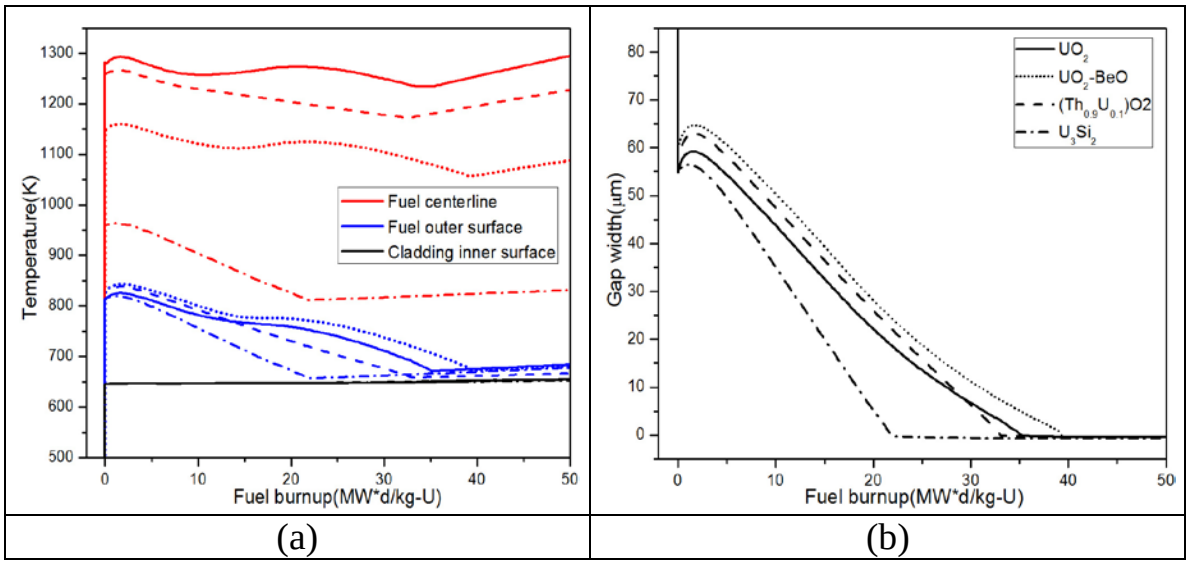


Figure 6 (a) Temperature at the fuel center (in red), outer surface (in blue) and cladding inner surface (in black). The solid line is for UO_2 fuel, dash line for $(Th_{0.9},U_{0.1})O_2$ fuel, dotted line for UO_2-10vol%BeO fuel and dash dotted line for U_3Si_2 fuel; (b) Gap size evolution for the four types of fuels. [20]

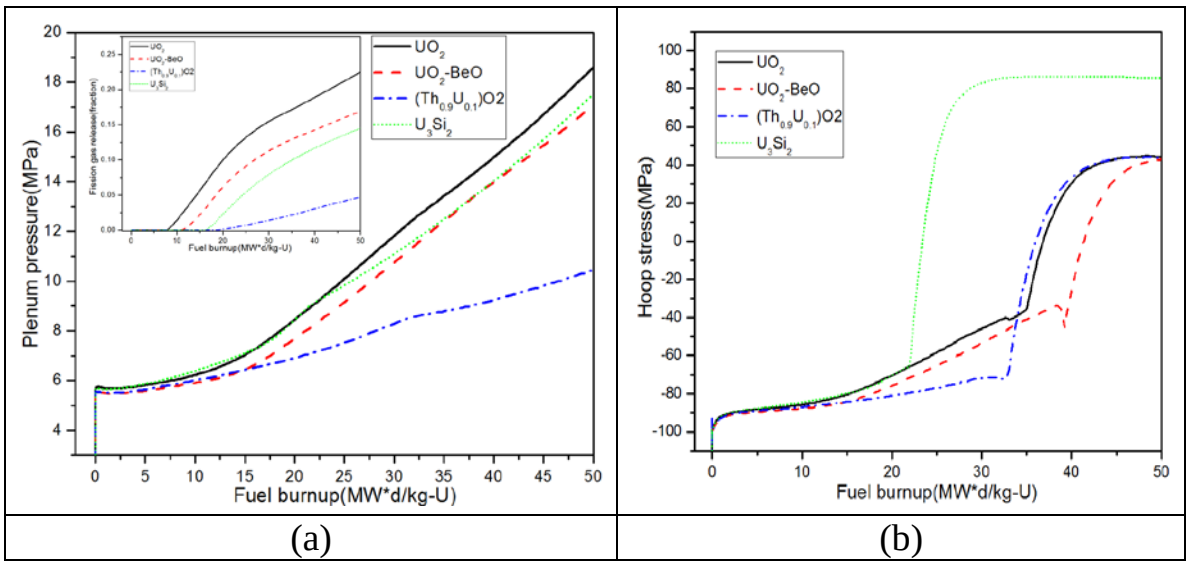


Figure 7 (a) Plenum pressure for the four types of fuels. Inset shows the corresponding fission gas release evolution. (b) Mid-pellet cladding hoop stress evolution of four types of fuels' cases with respect to fuel burnup. [20]

U_3Si_2 is the second lowest. The UO_2 fuel was found to have the highest plenum pressure and fission gas release fraction, while the composite fuel UO_2-10vol%BeO was found to effectively decrease the plenum pressure and fission gas release fraction (by lowering the temperature).

Finally, the cladding hoop stress at the mid pellet is shown in Figure 7(b). The hoop stress of U_3Si_2 fuel case was found to increase the most rapidly and had the largest final hoop stress. This may imply cladding over-strain could be an issue for this type of fuel. The UO_2, UO_2-10vol%BeO and $(Th_{0.9},U_{0.1})O_2$ fuel cases were found to have approximately the same value of hoop stress at the end of the burnup. For the UO_2-10vol%BeO and $(Th_{0.9},U_{0.1})O_2$ fuel cases, the increase in stress is manifested later. This is consistent with sequence of gap closure times.

The CAMPUS capability was further demonstrated by the development of a model for UO_2-SiC composite light water reactor fuel with enhanced thermal and mechanical properties to mitigate some of the material performance limitations. Hasselan and Johnson model was used to predict the UO_2-SiC composite thermal conductivity, and the predictions are in excellent agreement with the measured data.

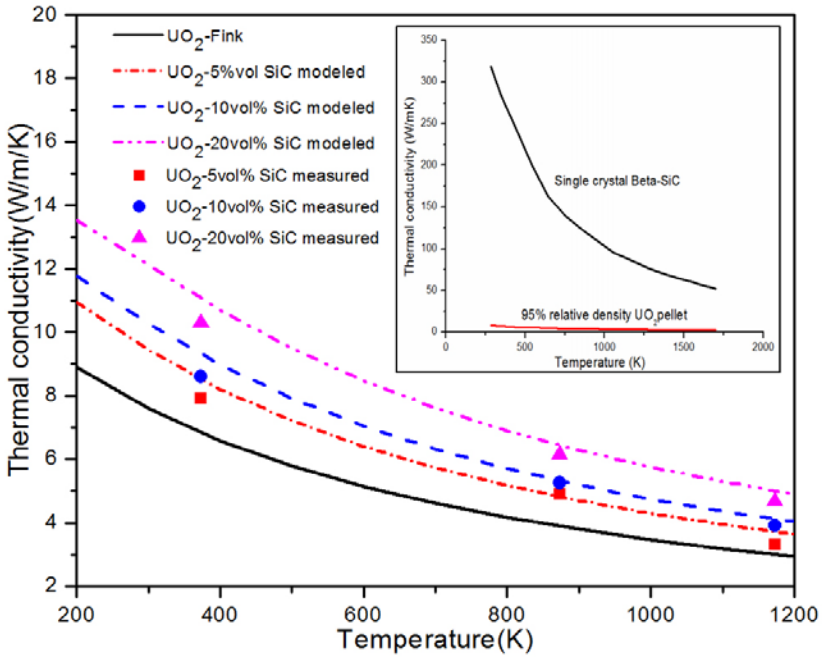
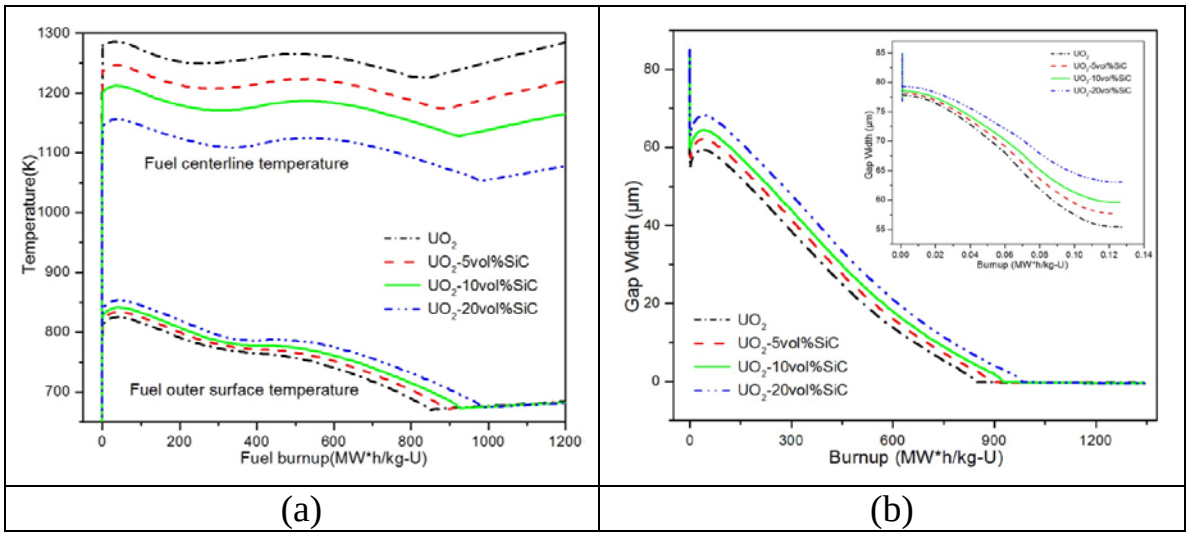


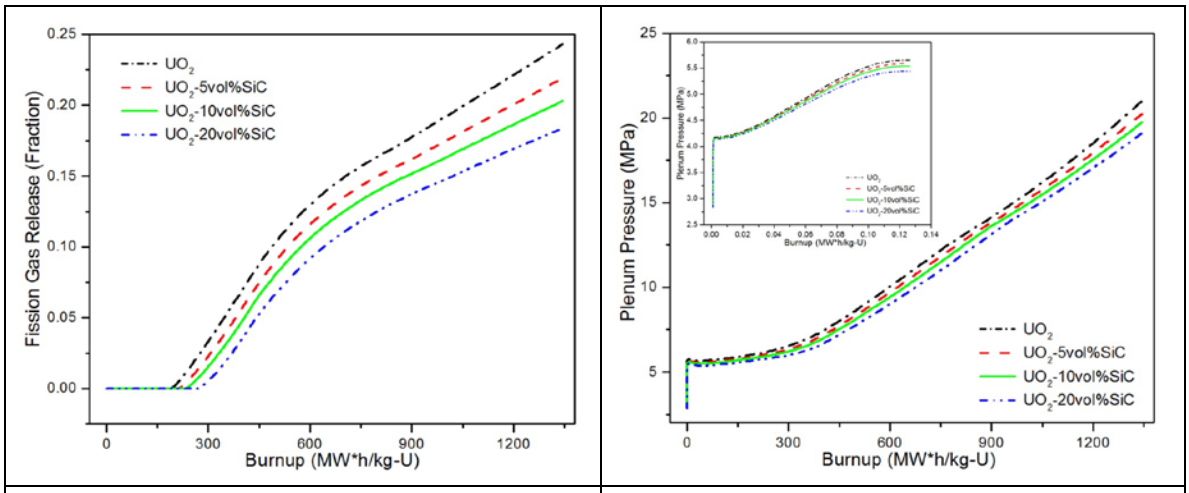
Figure 8 Thermal conductivity of UO_2 and UO_2-SiC fuels from measured and modeled results, inset shows comparison of thermal conductivities between UO_2 and beta SiC. [21]

From Figure 9(a), we can see that the fuel temperature can be significantly lowered using the enhanced thermal conductivity UO_2-SiC fuel. For the case of UO_2-20vol%SiC fuel and Zircaloy cladding, the fuel centerline temperature was lowered about 140 K compared to the UO2 fuel. However, there is no significant difference for UO2-SiC fuel outer surface temperature compared to UO2 fuel and Zircaloy cladding. The gap size evolution is shown in Figure 9 (b) for the four different cases: UO_2 fuel, UO_2-5vol%SiC fuel, UO_2-10vol%SiC fuel, and UO_2-20vol%SiC fuel. The gap size is a combined effect of fuel swelling, densification, thermal expansion and cladding creep down. From Figure 9(b), the closure of the gap is observed in order of increasing SiC content: UO_2, UO_2-5vol%SiC, UO_2-10vol%SiC and UO_2-20vol%SiC. The SiC addition not only increases the fuel thermal conductivity, which lowers the fuel temperature, but also lowers the volume fraction of the fuel to swell (which is significant for the fission gas swelling is non-linear with burnup).



(a) (b)

Figure 9 (a) Calculated temperature evolutions at fuel centerline, outer surface with: (1) UO_2 fuel and Zircaloy cladding; (2) UO_2-5vol%SiC fuel and Zircaloy cladding; (3) UO_2-10vol%SiC fuel and Zircaloy cladding; and (4) UO_2-20vol%SiC fuel and Zircaloy cladding. (b) Calculated gap size evolution with different type of fuels and Zircaloy cladding, inset shows the gap size evolutions of the first three hours. [21]



(a) **(b)**

Figure 10 (a) Calculated fission gas release evolution with different type of fuels and Zircaloy cladding. (b) Calculated plenum pressure evolution with different type of fuels and Zircaloy cladding, inset shows the plenum pressure evolutions of the first three hours. [21]

The fission gas release is depicted against fuel burnup in Figure 10(a) for the four different cases. The UO_2 case experienced the highest fission gas release fraction as expected due to its low thermal conductivity and

high fuel temperature. The fission gas release can be reduced by about 25% at the fuel burnup of about 1,200 MW*h/kg-U for UO_2-20vol%SiC fuel. For UO_2-5vol%SiC and UO_2-10vol%SiC fuel, the fission gas release can be reduced by around 10% and 17%, respectively, at the fuel burnup of about 1,200 MW*h/kg-U. Figure 10(a) also indicates that the earliest start time to release fission gas is found to be the case of UO_2 fuel without SiC addition. This is an expected observation as fission gas release is dominated by fuel temperature. Figure 10(b) shows the gap/plenum pressure evolution against fuel burnup for the four different cases (inset shows the evolution within the first three hours). Regular UO_2 fuel illustrates the highest gap/plenum pressure since its lower thermal conductivity leads to higher fuel temperature and more fission gas release. On the other hand, UO_2-20vol%SiC fuel and Zircaloy cladding experiences lowest gap/plenum pressure as shown in Figure 10(b).

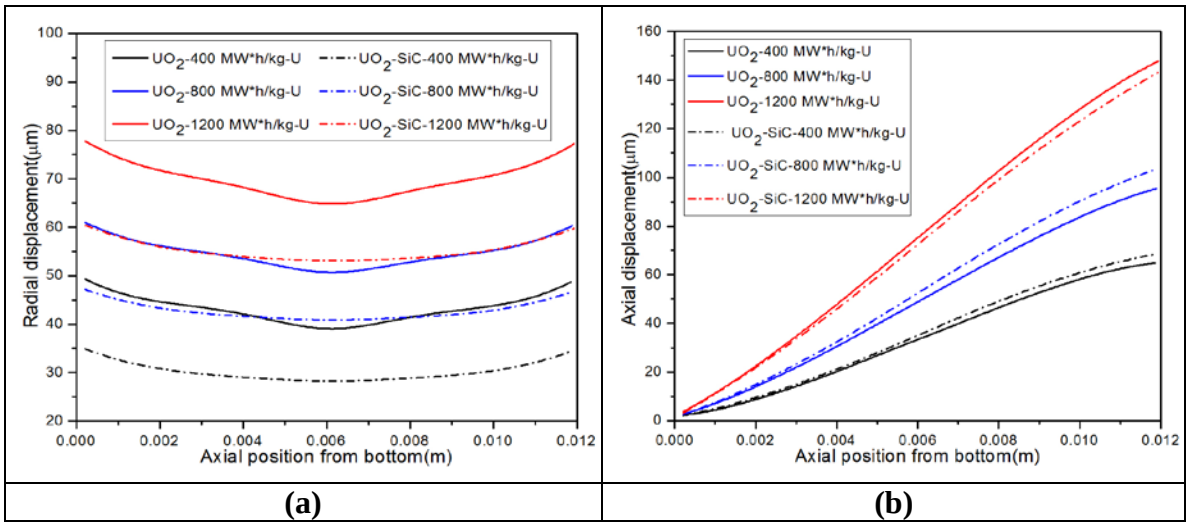


Figure 11 Calculated radial (a) and axial (b) displacement over the UO_2 and UO_2-20vol%SiC fuel surface at different fuel burnup. [21]

The radial and axial displacements are also depicted over the UO_2 and UO_2-20vol%SiC fuel surface at different fuel burnup, as shown in Figures 11(a)-(b). The radial displacement of UO_2 fuel is much larger than UO_2-20vol%SiC fuel, although both fuels types take on a so-called "hourglass" shape (i.e., the radial displacements at the fuel top and bottom are much larger than at the middle part of the fuel, which is caused by the elastic stress induced by the gradient in temperature field) while the fuel axial displacement is found to have significant difference.

5. Conclusions

An effective approach was developed using self-defined multiphysics models based on the framework of COMSOL Multiphysics to manage the nonlinearities associated with light water reactor fuels performance analysis. The modelling and simulations approach is of particular importance since it demonstrates highly interrelated and nonlinear fuel performance models can be developed and implemented into a multiphysics platform, and thus more efforts can be put into physics model development and improvement. The modelling results can be used to identify the important phenomena and parameters, to direct and design experiments and to assist in post analysis of expensive nuclear experiments for light water reactor nuclear fuel performance analysis.

6. References

[1] Hann, C.R., Beyer, C.E., Parchen, L.J., 1973. Gapcon-Thermal-1: A Computer Program for Calculating the GAP Conductance in Oxide Fuel Pins. Pacific Northwest Laboratories, Richland, WA.

[2] Rashid, Y., Dunham, R., Montgomery, R., 2004. Fuel analysis and licensing code: FALCON MOD01. EPRI Report 1011308.

[3] Nakajima, T., Saito, H., Osaka, T., 1994. FEMAXI-IV: A computer code for the analysis of thermal and mechanical behavior of light water reactor fuel rods. Nucl. Eng. Des. 148(1), 41-52.

[4] Berna, G.A., Beyer, C.E., Davis, K.L., Lanning, D.D., 1997. FRAPCON-3: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burn-up. NUREG/CR-6534, Idaho National Engineering and Environmental Laboratory.

[5] Geelhood, K.J., Luscher, W.G., Beyer, C.E., Cuta, J.M., 2011. FRAPTRAN 1.4: A Computer Code for the Transient Analysis of Oxide Fuel Rods. NUREG/CR-7023, Pacific Northwest Laboratories, Richland, WA.

[6] Bentejac, F., Hourdequin, N., 2004. TOUTATIS: an application of the CAST3M finite element code for PCI three-dimensional modeling. Proceedings of Pellet–Clad Interaction in Water Reactor Fuels, 495–506, Aix-en-Provence, France.

[7] Thouvenin, G., Michel, B., Sercombe, J., 2007. Multidimensional modeling of a ramp test with the PWR fuel performance code ALCYONE. Proceedings of the 2007 International LWR Fuel Performance Meeting, San Francisco, California.

[8] Williamson, R.L., Hales, J.D., Novascone, S.R., Tonks, M.R., Gaston, D.R., Permann, C.J., Andrs, D., Martineau, R.C., 2012. Multidimensional multiphysics simulation of nuclear fuel behavior. J. Nucl. Mater. 423(1–3), 149-163.

[9] Hales, J.D., Novascone, S., Pastore, G., Perez, D., Spencer, B., Williamson, R., 2014. BISON Theory Manual: The Equations behind Nuclear Fuel Analysis, Fuels Modeling & Simulation Department, Idaho National Laboratory, Idaho Falls, Idaho.

[10] Gamble, K., Williams, A.F., Chan, P.K., Wowk, D., 2015. HORSE: A simulation tool for modeling three-dimensional deformation in CANDU reactor fuel elements. Nucl. Eng. Des. 293, 385-394.

[11] Williamson, R.L., 2011. Enhancing the ABAQUS thermomechanics code to simulate multipellet steady and transient LWR fuel rod behavior. J. Nucl. Mater. 415(1), 74-83.

[12] Prudil, A., Lewis, B.J., Chan, P.K., Baschuk, J.J., 2015. Development and testing of the FAST fuel performance code: Normal operating conditions (Part 1). Nucl. Eng. Des. 282(0), 158-168.

[13] Prudil, A., Lewis, B.J., Chan, P.K., Baschuk, J.J., Wowk, D., 2015. Development and testing of the FAST fuel performance code: Transient conditions (Part 2). Nucl. Eng. Des. 282(0), 169-177.

[14] Notley, M.J.F., 1979. ELESIM: A computer code for predicting the performance of nuclear fuel elements. Nucl. Technol. 44 (3), 445-450.

[15] Chassie, G.G., Sim, K.S., Wong, B., Papayiannis, G., "ELESTERS code Upgrades", The 9th International Conference on CANDU Fuel, Bellville, 2005.

[16] Williams, A.F., "The ELOCA Fuel Modelling Code: Past, Present and Future," The 9th International Conference on CANDU Fuel, Belleville, 2005.

[17] Prudil, A., 2014. FAST: A Fuel And Sheath modeling Tool for CANDU Fuel. PhD Thesis, Royal Military College of Canada, Kingston, Canada.

[18] Allison, C.M., Berna, G.A., Chambers, R., Coryell, E.W., Davis, K.L., Hagrman, D.L., Hagrman, D.T., Hampton, N.L., Hohorst, J.K., Mason, R.E., McComas, M.L., McNeil, K.A., Miller, R.L., Olsen, C.S., Reymann, G.A., Siefken, L.J., 1993. SCDAP/RELAP5/MOD3.1 code manual volume IV: MATPRO. Technical Report NUREG/CR-6150, Idaho National Laboratory.

[19] Liu, R., Zhou, W., Shen, P., Prudil, A., Chan, P.K., 2015. Fully Coupled Multiphysics Modeling of Enhanced Thermal Conductivity UO_2-BeO Fuel Performance in a Light Water Reactor. Nucl. Eng. Des. 295, 511–523.

[20] Liu, R., Prudil, A., Zhou, W., Chan, P.K., 2016. Multiphysics Coupled Modeling of Light Water Reactor Fuel Performance, Prog. Nucl. Energ. 91, 38-48.

[21] Liu, R., Zhou, W., Prudil, A., Chan, P.K., Multiphysics modeling of UO_2-SiC composite fuel performance with enhanced thermal and mechanical properties, Appl. Therm. Eng. revised version under review.