Development of Terrenus: A Multiphysics Code for Spent Nuclear Fuel Canister Criticality Analysis[1]

Gregory G. Davidson,* Seth R. Johnson,* Stylianos Chatzidakis†

*Radiation Transport Group
†Used Nuclear Fuel Group
Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN,
davidsongg@ornl.gov, johnsonsr@ornl.gov, chatzidakiss@ornl.gov

INTRODUCTION

This is a technical paper that does not take into account contractual limitations or obligations under the Standard Contract for Disposal of Spent Nuclear Fuel and/or High-Level Radioactive Waste (Standard Contract) (10 CFR Part 961). For example, under the provisions of the Standard Contract, spent nuclear fuel in multi-assembly canisters is not an acceptable waste form, absent a mutually agreed to contract amendment. To the extent discussions or recommendations in this paper conflict with the provisions of the Standard Contract, the Standard Contract governs the obligations of the parties, and this paper in no manner supersedes, overrides, or amends the Standard Contract.

This paper reflects technical work which could support future decision making by DOE. No inferences should be drawn from this paper regarding future actions by DOE, which are limited both by the terms of the Standard Contract and a lack of Congressional appropriations for the Department to fulfill its obligations under the Nuclear Waste Policy Act including licensing and construction of a spent nuclear fuel repository.

A new multiphysics code, *Terrenus*, is in development at Oak Ridge National Laboratory (ORNL). The purpose of Terrenus is to simulate the consequences of a spent nuclear fuel (SNF) dual purpose (storage and transportation) canister (DPC) entering a critical configuration while in a geological repository, including calculating heat generation, pressure buildup, and increase in radionuclide inventories.

Subcritical configuration in loaded SNF DPCs is usually maintained by using neutron absorber panels placed between fuel assemblies. These absorbers are typically composed of boron carbide and aluminum. Since repository periods of interest are at least 10,000 years long, it is unlikely that aluminum-based absorbers will maintain criticality control for that amount of time in an aqueous environment. Many currently loaded DPCs may achieve criticality under certain conditions (e.g., loss of absorber panels in a flooded scenario) over a repository time frame [1]. Therefore, consequence of a DPC criticality event in a geological repository is being investigated to determine the feasibility of direct disposal of DPCs.

The simulation software suite will be composed of four components: a radiation transport code, a depletion code, a thermal hydraulics solver, and a structural simulation code. The radiation transport code is Shift [2], a high-performance Monte Carlo code developed at ORNL, which will calculate heat generation in the fuel rods. The evolving nuclide inventory will be calculated by ORIGEN, a nuclide burnup and decay solver in SCALE [3]. The thermohydraulic solver is COBRA-SFS Cycle 4a [4]. COBRA-SFS solves subchannel equations to compute the pressure, density, and temperature in the system. Finally, the structural code to be used is Diablo, a three-dimensional structural-thermal-mechanics code. Diablo [5] will be used to calculate the stress, strain, and deformation on the cask vessel and structural internals.

Initial development is focused on coupling Shift and COBRA-SFS for steady-state coupled transport-thermohydraulic simulations. A series of challenge problems is being developed, beginning with steady-state coupled transport-thermal hydraulics simulations of a 3×3 array of pins, eventually proceeding up to time-dependent coupled simulations of fully loaded DPCs. This paper demonstrates the results of the initial efforts in steady-state coupled transport and thermal hydraulics applied to a 3×3 array of pins in a flooded spent-fuel canister. This work was originally published in Ref. [6].

COUPLED CODES

The Terrenus framework currently couples the Shift Monte Carlo code to the COBRA-SFS thermal hydraulics code. Shift is used to calculate reactivity and power distribution of SNF within a canister, while COBRA-SFS is used to calculate thermal hydraulic and quantities such as fluid density and temperature, as well as heat transfer between the fuel pins and surrounding channels. Details of Shift, COBRA-SFS, and the Terrenus coupling code are given below.

Shift

Shift is a high-performance, massively parallel Monte Carlo code featuring both continuous-energy and multigroup physics. Shift is capable of solving problems in both k-eigenvalue and fixed-source modes [2]. Shift can model coupled neutron/photon physics, including secondary particles born both by collisions and fission, and it features on-the-fly Doppler broadening for calculating cross sections at precise temperatures, an important capability for high-fidelity neutronic-thermal hydraulic coupling.

Shift has excellent scaling up to leadership-class supercomputers, and it features domain decomposition, which enables is to simulate large problems. A fully loaded DPC canister can

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hold as many as 40 pressurized water reactor (PWR) assemblies, making criticality simulations of DPCs relatively large and challenging problems. Since Shift has previously been used by the Consortium for Light Water Reactors (CASL) as part of the VERA code to perform excore analysis of full PWR models [7], it is anticipated that Shift will also have the capacity to model DPCs.

COBRA-SFS

COBRA-SFS is a program for steady-state and transient simulation of the thermal-hydraulic behavior of SNF systems [4]. Similar to other codes in the COBRA family—such as COBRA-TF [8]—COBRA-SFS solves a set of subchannel equations describing conservation of mass and momentum in the coolant flowing within fuel assemblies, as well as energy conservation within the fuel rods and other solid structures in the system. COBRA-SFS retains the validation history of other codes in the COBRA series, but it also provides additional validation specific to analysis of spent fuel systems [9]. COBRA-SFS is distinguished from other COBRA variants by its treatment of features specific to spent fuel storage systems. This includes the ability to model natural circulation of coolant within a fuel cask, as well as simulation of radiative heat transfer between fuel rods and solid structures such as a spent fuel cask. It also extends the iteration scheme of other COBRA versions to be fully implicit in time, allowing stronger coupling between equations governing fluid energy and heat transfer in solid components of the system.

Terrenus

Terrenus is the code responsible for coupling Shift and COBRA-SFS; this requires overcoming several technical hurdles. The primary difficulty is designing an efficient interface between a serial, I/O-based process (COBRA-SFS) and a massively parallel framework (Shift). Shift has a comparatively large startup cost due to the loading of the nuclear data from disk, so it is desirable to provide Shift an in-memory interface that allows the Shift processes to remain active but idle while COBRA-SFS generates updated thermal hydraulics data. A Python-based driver code that launches and coordinates the Shift and COBRA-SFS processes achieves this design goal.

The Python driver code has three main responsibilities: interaction with COBRA-SFS, interaction with Shift, and coordination between the two. Since COBRA-SFS uses a fixed-column input format and human-readable output format, the driver must be able to generate text-based fixed-column input from numerical data. The input format for COBRA-SFS has several limitations that affect the accuracy of the simulation, the most significant of which is that COBRA-SFS's input allows only an axial power profile and a separate radial power profile, implying that the 3-D power distribution calculated by Shift must be approximated by a separable function in r and z. An additional limitation is in the fixed-column input format: most variables must be represented in fixed-point notation inside five or ten columns, limiting both the accuracy and the range of values that can be provided to COBRA-SFS. Finally, since COBRA-SFS uses the imperial system of units, care must be taken to properly convert values to and from Shift's results. To ensure the validity of the conversions, the Python driver parses the units of each field in the output and uses an open source unit conversion package (*pint*) to maintain the integrity of the units through the code.

Shift's application program interface (API) uses a parallel HDF5-format interface to efficiently read, distribute, and write thermal hydraulic and neutronics data. Since it has this computer-readable metadata-rich I/O interface, robustly providing input and reading output from Shift are comparatively simple tasks. The challenge of coupling to Shift is informing the code when new input is available, and determining when newly generated output can be safely read. This is overcome using special command tokens piped through the standard input and output streams between the Shift MPI executable and the Python driver code.

The final task for the Python driver is to asynchronously run and coordinate the COBRA-SFS and Shift processes. These processes run independently using Python's *asyncio* module, which allows the driver process to interleave input, output, and command execution between the two codes. This, for example, allows processing of the COBRA-SFS output file to complete while Shift is still solving the neutronics. When Shift reports convergence, or if either code fails unexpectedly, then the driver cleanly terminates both codes.

RESULTS

Terrenus is currently capable of modeling any single PWR assembly within a canister, including fuel pins and guide tubes. Capabilities necessary for multiple assemblies have not yet been implemented. To demonstrate the code, a stainless steel box containing a 3×3 array of PWR fuel pins was simulated, as shown in Fig. 1.

The fuel rod definitions are taken from Godfrey [10]. The fuel pin radius is 0.4096 cm, the inner clad radius is 0.418 cm, and the outer clad radius is 0.475 cm. The active fuel height is 365.76 cm, and the pin pitch is 1.26 cm. No spacer grids were modeled. The fuel was modeled as fresh 3.1 wt% enriched UO_2, the gap was modeled as helium, and the clad was modeled as Zircaloy-4. The DPC was modeled as fully flooded with pure water. The details of the fuel, gap, and cladding compositions are given in Godfrey's report [10], and a gap conductance of 0.6469 W/m K was used. The fission heat was calculated at 18 evenly spaced axial levels along the height of the assembly. A total power of 100 W was assumed. The outer boundary was assumed to be fixed at an ambient temperature of 60 degrees Fahrenheit. As shown in Fig. 1, the array was held in a stainless steel box with thickness of 1 cm.

For COBRA-SFS, the DPC cask walls were modeled explicitly, whereas with Shift, reflecting boundaries were set radially around the 3×3 array of pins. This was done to give the pincell array a higher reactivity that would be more similar to what would be experienced by a fully loaded cask. Thermal properties of the fuel rods and surrounding water are given in Tables I and II, respectively.

The radiation transport and thermal hydraulics were allowed to iterate for 10 iterations. A convergence criteria of 10^{-3} was imposed on the fission power, which was calculated

TABLE I. Thermal properties for fuel

Fuel cond. [W/m K]	Fuel sp. heat [J/g K]	Fuel density [g/cm^3]	Pellet diam. [cm]	Clad cond. [W/m K]	Clad sp. heat [J/g K]	Clad density [g/cm^3]	Clad thick. [cm]
5.1887	0.247	10.492	0.8189	17.2958	0.419	6.552	0.5692

TABLE II. Thermal properties for water

Temp [K]	Enthalpy [J/g]	Conduction [W/m K]	Sp. heat [J/g K]	Sp. volume [ft^3/lbm]	Viscosity [g/m s]
277.6	18.61	0.5690	4.1868	0.9988	1.5477
288.8	65.13	0.5898	4.1868	0.9988	1.1203
300.0	111.65	0.6088	4.1868	1.0051	0.8570
322.0	204.69	0.6417	4.1868	1.0113	0.5564
344.3	297.73	0.6642	4.1868	1.0238	0.3973
355.4	344.25	0.6711	4.1868	1.0301	0.3452
366.5	390.77	0.6763	4.1868	1.0363	0.3018

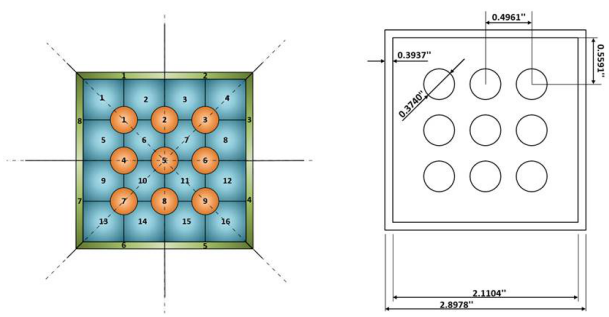

Fig. 1. Schematic representation of 3×3 square array of spent fuel rods within a canister. The left image shows the COBRA-SFS channel, rod, and slab nodalization, while the right image shows the dimensions.

by the Shift. However, it was found that the stochastic nature of the radiation transport solver caused non-monotonic statistical behavior in the fission power, so the calculation appeared to never converge. This was actually not the case, however, as shown in the results below. In the future, a convergence condition on the channel temperature and density fields will be developed. Since these are calculated from a deterministic subchannel computation, these fields are expected to be much more stable and therefore more appropriate for measuring convergence.

The powers were under-relaxed before being communicated to the subchannel code using

$$P^{(i+1)} = fP^{(i+1,*)} + (1-f)P^{i}, \tag{1}$$

where $P^{(i+1)}$ is the power at time $i+1$, $P^{(i+1,*)}$ is the just-calculated power from the radiation transport code, and f is the under-relaxation factor. Multiphysics simulations are nonlinear, and fixed-point coupling can often cause a given physics simulator to over-shoot the converged solution, thereby increasing the number of iterations necessary and reducing computational performance. For the simulation results given below, a factor of 0.7 was used. Future work will include a study to find the optimal under-relaxation parameter for various problems of interest.

For each iteration, a Monte Carlo radiation transport simulation was performed with 1,000 total cycles, 25 inactive cycles, and 10,000 histories per cycle. Fission power was calculated using a mesh tally placed over the pin cell boundaries spanning 18 evenly spaced axial levels. Energy released per fission was calculated using the values in the ENDF-VII.1 libraries [11], which are 194.02 MeV/fission in ^{235}U and 198.122 MeV/fission in ^{238}U. Because COBRA-SFS does not support radiative heating in the channel, gamma heating was neglected. Future calculations could compute the gamma heating to better understand the consequence of this assumption.

Figure 2 (*left*) shows the radial power distribution for iteration 1 at the midplane z = 185 cm of the 3×3 geometry. Physically, the power distribution should be perfectly flat, and within some statistical variation, this is what was found. Figure 2 (*right*) shows the power in the central pin at the axial midplane over 10 iterations. The power appears to hit an asymptote at around iteration 5, but convergence is difficult to ascertain due to the statistical variations in the Monte Carlo power calculation.

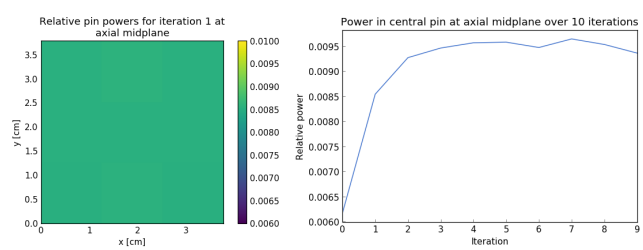

Fig. 2. Pin powers at axial midplane for iteration 1 (*left*) and power in central pin at axial midplane over 10 iterations (*right*).

Figure 3 (*left*) shows the channel temperatures for iterations 1 through 3 at the axial midplane, illustrating that channel temperatures appear to converge quickly. This suggests, as mentioned above, that the multiphysics simulation should be converged on channel properties rather than pin powers since these are more numerically stable. As expected, the inner chan-

nels are at a higher temperature since they are not adjacent to the cooler ambient temperature. Figure 3 (*right*) shows the axial distribution of the temperature in one of the central channels over four iterations. It can be seen that channel temperatures quickly converge and behave as expected, with a rising temperature along the axial length of the fuel until near the top of the assembly, where the water encounters the cooler ambient temperature at the boundary.

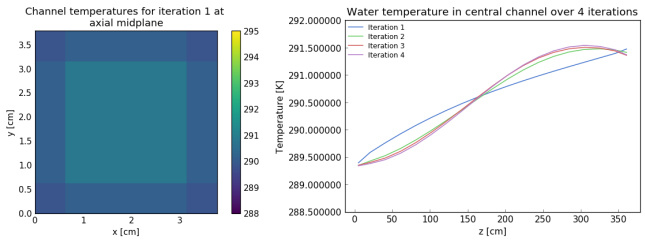

Fig. 3. Radial channel temperatures at axial midplane for iteration 1 (*left*) and temperature in a central channel at axial midplane over 4 iterations (*right*).

Figure 4 (*left*) shows the channel water densities. As with the channel temperatures, rapid convergence is seen. As expected, there is an inverse relationship between density and temperature, with lower densities in the center channels where the water is hottest, and higher densities near the boundary where it is coolest. Figure 4 (*right*) presents the axial water density distribution in a central channel. As expected, the density of the water is reduced as the temperature increases up the channel until near the top, where the water begins to be cooled by the cooler top boundary condition. As before, the axial density distribution converges rapidly.

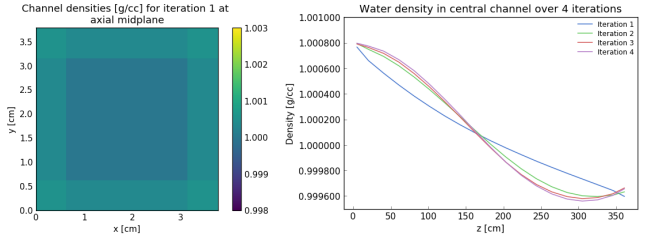

Fig. 4. Radial channel densities at axial midplane for iteration 1 (*left*) and density in a central channel at axial midplane over 4 iterations (*right*).

CONCLUSIONS AND FUTURE WORK

An initial multiphysics framework—Terrenus—has been developed to couple Monte Carlo radiation transport code Shift and thermal hydraulics code COBRA-SFS. Currently, the Terrenus code is capable of coupling Shift and COBRA-SFS for a simplified cask model containing a single PWR assembly. The Terrenus framework has been tested using a simplified 3×3 fuel pin geometry.

Future work will expand the geometric capabilities of Terrenus so that a full cask of arbitrary reactor assemblies can be modeled, as well as the cask internals. This will require adding an assembly-aware metadata layer onto generalized geometry package within Shift and will require a much more general-purpose COBRA-SFS input template, as well.

Finally, Terrenus currently requires the user to specify the total power of the system. Future work will include enabling Terrenus to calculate the negative temperature coefficient of the cask system so that a critical temperature search can be performed. The coupled transport thermohydraulics system will be able to iterate to the actual power. A new convergence criterion which uses the more stable thermohydraulics parameters (channel temperature and density) rather than the stochastically noisy radiation transport parameter (power) will also be developed.

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