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Two-Dimensional Modeling of Spent Nuclear Fuel Using FLUENT

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***Abstract*—**In a nuclear reactor, an array of fuel rods containing stacked uranium dioxide pellets clad with zircalloy is the heat source for a thermodynamic cycle of energy conversion from heat to electricity. After fuel is used in a nuclear reactor, the assemblies are stored underwater in a spent nuclear fuel pool at the nuclear power plant while heat generation and radioactive decay rates decrease before it is placed in packages for dry storage or transportation. A computational model of a Boiling Water Reactor spent fuel assembly is modeled using FLUENT, the computational fluid dynamics package. Heat transfer simulations were performed on the two-dimensional 9x9 spent fuel assembly to predict the maximum cladding temperature for different input to the FLUENT model. Uncertainty quantification is used to predict the heat transfer and the maximum temperature profile inside the assembly.

***Keywords*—**Spent nuclear fuel, conduction, heat transfer, uncertainty quantification.

I. Introduction

ONE of the primary methods to run a nuclear power cycle is to use a Boiling Water Reactor (BWR). In a BWR setup, uranium dioxide (UO_2) is used as fuel. The fuel compounds are manufactured into pellets that are placed inside a zircalloy cladded tube before they are sealed. Once sealed, the fuel tubes are interspersed in a column where water passes over. The heat radiated away from the fuel pellets boils the surrounding water until it evaporates into steam. The steam is then run through turbines generating power similar to natural gas thermodynamic power cycles.

Once the fuel has decayed enough to low heat generation levels, the rods containing the fuel are removed and placed into a storage assembly. The storage assemblies range between 7x7, 9x9, 13x13, and 14x14 configurations that hold the spent fuel rods [1], [2]. The specific geometries are contingent upon the manufacturer of the assembly. This study concerns itself with the 9x9 configuration produced by General Electric.

After the fuel is sealed in the storage assembly, it is typically transported to a wet storage facility where the assembly will radiate heat in a pool to dissipate the release of energy. After spending years in the spent fuel pool, the assembly is removed from the pool and moved into a dry storage cask. In a package, individual fuel assemblies are stacked inside the cask containment volume. The containment region is evacuated and back-filled with helium, a high thermal conductivity gas that is slightly-pressurized to induce a higher convective heat transfer rate [3]. The concern of this research is to simulate the heat transfer mechanics that occur within the assemblies and casks. The typical cladding material, zircalloy, experiences a structural weakening at approximately 400 °C, a temperature that the fuel must be maintained below to avoid high hoop stress [4]. At this temperature, it is possible for the assemblies to emit harmful radiation to the outside environment. Additionally, it is not possible to open an assembly to measure temperature as this would also release harmful radiation. It is useful to simulate the conditions that the fuel assemblies experience to obtain numerical values for temperature.

To account for random fluctuations in natural systems, this study has included a sensitivity analysis that uses Uncertainty Quantification (UQ) methods. UQ methods applied to a computationally accurate model provide a more complete picture of the potential temperatures inside of the assemblies.

This research specifically aims at investigating the effects of different geometries, anisotropic material construction, and chaotic variables on the heat transfer inside Spent Nuclear Fuel (SNF) casks.

The computation relies on creating a geometrically coherent mesh that leads to smooth nodal calculations that represent a realistic heat transfer model.

One overlooked element of the simulation is whether or not the fuel clad emissivity strongly affects temperature distribution. Emissivity is one important characteristic that describes how much energy a material or surface releases [5]. This study will examine not only varying geometry and material types for critical components, such as cladding and cask walls, but it will also investigate the effects of emissivity of such components. Many researchers in this field have looked at the heat transfer inside the assemblies [6], [7] by looking at the uncertainty of the input parameters one at a time. The novelty in our modeling techniques is the ability to study the uncertainty of all input parameters at the same time.

This study will use ANSYS and Fluent to create a two-dimensional geometry of the SNF cask. A three-dimensional Fluent model will not be possible to simulate using a desktop computer unless an effective thermal conductivity model is used [8].

This study will focus on a 9x9 zircalloy cladding of UO_2 pellets with a Helium backfill enclosed by a zircalloy, water

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neutron-shield, and steel cask wall. These simulations and iterations in the FLUENT engine will be controlled by a user-defined function that is written in a MATLAB code iterating over various changes in controllable boundary conditions. Emissivity and other material properties may be tested over the iterations to isolate specific instances of critical temperature or pressure loadings inside the SNF cask.

II. Uncertainty Quantification

UQ is a mathematical tool for examining the effect of uncertainty in input parameters to a model, and their subsequent effect on the outputs.

Due to the complexity of the materials and construction involved with SNF storage, there is a substantial amount of uncertainty on the material properties; these properties serve as inputs to a physical model. However, because of the amount of materials used, performing a parametric analysis would be extremely time consuming and costly.

UQ gives the ability to examine the effect of these uncertainties on the outcome of the model.

A simplified model of the process can be presented as:

$$Y = F(X)$$

X is a one-dimensional input parameter; F, which takes X, is an example of a model, and Y is the output of the model. In our case X could be the thermal conductivity of the buffer gas He, F would be our ANSYS FLUENT CFD model, and Y could be the velocity, pressure, or temperature throughout the model.

Both the input variable and output variable can be expressed by a polynomial expansion:

$$\sum_{i=0}^{p} y_i \psi_i(\xi) = F\big(X(\xi)\big), \quad X(\xi) = \sum_{i=0}^{q} x_i \psi_i(\xi)$$

where ψ are *Legendre Polynomials*, ξ is a random variable quadrature, p is Highest order expansion, and *x,y* are the PCE coefficients.

Sensitivity analysis is performed by acquiring the output PCE coefficients, y_i in the example above. This is done through Non-Intrusive Spectral Projection (NISP).

Given the orthogonality of Legendre Polynomials, the coefficients *y* are given by,

$$y_i = \frac{<F(X)\psi_i>}{<\psi_i^2>}$$

where *F(X)* represents the actual model solutions of temperature in the mesh.

For multivariate simulations, i.e. simulations that have more than one uncertain input parameter, the formalism takes on several adjustments. Instead of a single random variable quadrature, there is a multidimensional quadrature, and therefore a multidimensional polynomial basis. Furthermore, the number of terms in the polynomial expansion is given by,

$$N_{pc} = \frac{(n+p)!}{n!p!}$$

where p still represents the highest order polynomial (abbreviated, N-ord), and n represents the number of stochastic dimensions (N-dim).

The assignment of the polynomial terms relies on the existence of a 'multi-index',

$$M_i^j = l$$

where j corresponds to the dimension of interest, i corresponds to the term out of N_{pc}, and l corresponds to the polynomial term in the multidimensional expansion.

This allows us to transform the univariate expansion into the multivariate case,

$$\sum_{i=0}^{p} x_i \psi_i(\xi) \rightarrow \sum_{i=0}^{N_{pc}} x_i \Psi_i(\mathrm{E})$$

Here it should be noted that E represents the multi-dimensional quadrature, which is now a matrix instead of a vector as in the univariate case. The multidimensional polynomial basis is produced through,

$$\Psi_i(\mathrm{E}) = \prod_{j=1}^{n} \psi_l^j(\xi^j) \; where \; l = M_i^j$$

III Fluent Model

We used FLUENT CFD package by ANSYS 17.0 [9] to perform the simulations for this study. Fig. 1 shows the two-dimensional model composed of 44,187 elements and representing the cross-section of a 9x9 fuel rod array stored with the rods parallel to the ground. In this configuration, gravity is in the negative y direction. The rods are made up of a UO_2 core surrounded by a zircalloy-2 sheath. The rod array is centered within a stainless-steel enclosure.

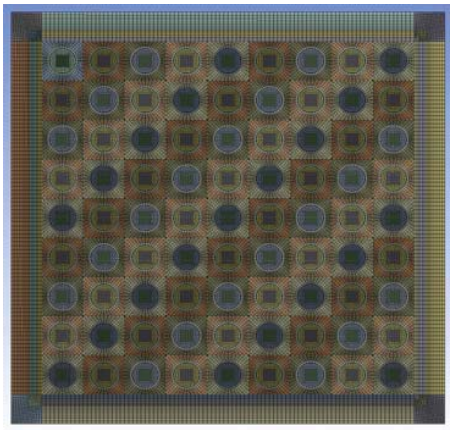

Fig. 1 Computational FLUENT Mesh

The heat is generated within the UO_2 cores and transferred to the outer wall of the assembly through conduction, convection and radiation. The stochastic dimensions are presented in Table I.

The heat transfer modes considered in the simulations are convection, surface-to-surface conduction, and radiation. Gases

participate in radiative heat transfer mechanics in the scope of this study. We fixed the temperature of the outer wall of the assembly for the scope of this study. Also, we considered gravity in the negative y-direction which contributed to the convective heat transfer.

TABLE I
VARIABLES PARAMETERS

Variable	Description	Units
He K	Helium Thermal conductivity	W/m·K
He Cp	Helium Specific Heat	J/kg·K
Zr K	Zircalloy Thermal conductivity	W/m·K
Zr Cp	Zircalloy Specific Heat	J/kg·K
ZrEm	Zircalloy Emissivity	
UO_2 K	Uranium Thermal conductivity	W/m·K
UO_2 Cp	Uranium Specific Heat	J/kg·K
Wall T	Wall Temperature	Kelvin
Power	Fuel Heat Generation	W/m^2
Fuel Em	Fuel Emissivity	
He K	Helium Thermal conductivity	W/m·K
He Cp	Helium Specific Heat	J/kg·K
Zr K	Zircalloy Thermal conductivity	W/m·K
Zr Cp	Zircalloy Specific Heat	J/kg·K
ZrEm	Zircalloy Emissivity	

The thermal fluid dynamic analysis of the assembly used the FLUENT 17.0 solver to provide the numerical solutions to the Navier-Stokes Equations. Reynolds Averaged Navier-Stokes method was used in this laminar model.

All of the UQ mathematics were handled through the MATLAB release of the Sandia National Labs UQToolkit, any further formalism is beyond the scope of this paper [10], [11].

Although ANSYS - FLUENT was used for the modeling of the storage container, MATLAB was used for the combination of the UQ methodology with the superior CFD capabilities of ANSYS. We developed a robust procedure to create and combine case files and solution files from ANSYS, and complete the UQ analysis in the MATLAB environment.

The uncertainty of each parameter is treated as input to the MATLAB program. The UQToolkit is able to create a multivariate quadrature of multiple parameters; each set of parameters represents a different CFD simulation. These parameters are mapped together and then directed into a batch of Fluent commands. Fluent will run thousands of simulations, each time producing solution data such as total temperature, velocity, and pressure. These solution files are then automatically imported into MATLAB and used in UQ analyses. These novel programs have provided a link between MATLAB and ANSYS - Fluent. This link is model-dependent, and relies on a pre-composed dictionary of fluent commands which can be created using the ANSYS – Fluent user interface. The user can specify uncertainty parameters and commence a batch-mode style series of simulations which ANSYS performs. The simulation files are then collected by MATLAB and prepared for analysis.

III. SENSITIVITY ANALYSIS

The first analysis performed was a sensitivity analysis for the input parameters. With ten stochastic inputs to our Fluent model (Ndim = 10), a first order Legendre Polynomial (Nord = 1) was used in the UQ calculations to generate the quadrature-dependent values for each variable.

The variable parameters, and their mean values, are in Table II. The uncertainty in each value is assumed to be ±10% with the special exception of the boundary temperature at the wall of the Stainless Steel basket, this was modeled over a range of 100 K from 50 ºC to 150 ºC, these were selected to cover a range of possible ambient temperatures inside the storage facility. Also note we have control over modeling the effective age of the UO_2 pellets by changing the Power source-term of the material to be varying ±10% about a higher or lower mean value.

TABLE II
INPUT VARIABLES FOR NDIM10 NORD1

Variable	Mean
He Cp	5192.5
Zr K	15
Zr Cp	300
ZrEm	0.9
UO_2 K	5
UO_2 Cp	235.15
Wall T (K)	373
Power	30000
Fuel Em	0.9

To generate the data needed for the sensitivity analysis, 1,024 FLUENT simulations were run using data from the multivariate quadrature generated in MATLAB. The wall time on the local machine with Intel Xeon E3, 3.50GHz cores, was approximately 15 hours.

In most cases, the coefficients of the center-temperature expansion were orders of magnitude less than their nominal uncertainty ranges. The two most contributing terms are seen to be the boundary Wall Temperature, and the Power term.

IV. RESULTS

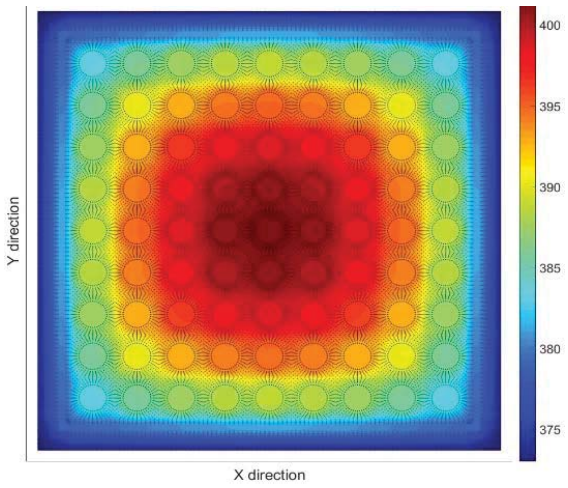

Fig. 2 Temperature Distribution

Fig. 2 shows a sample of the mean temperature distribution

of the temperature inside the fuel assembly (in Kelvin) for the 1024 simulations of dimension ten and Legendre Polynomial order of one. The wall temperature is a fixed boundary condition while the fuel rods inside the assembly are generating heat during dry storage which causes the center of the assembly to have the maximum temperature.

Fig. 3 shows the Probability Density Function of the temperature at the center of the 9x9 assembly.

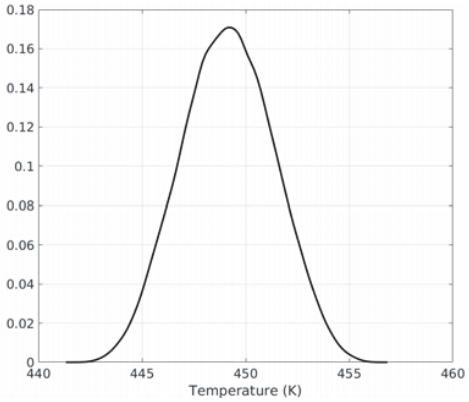

Fig. 3 PDF of the center temperature

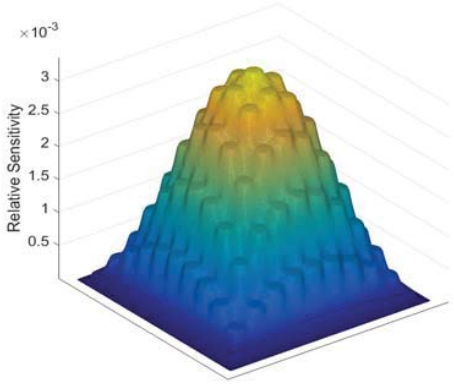

Fig. 4 Surface of Temperature Sensitivity to Fuel Power

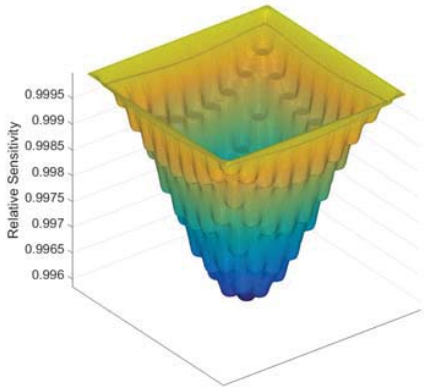

Fig. 5 Surface of Temperature Sensitivity to Boundary Wall Temperature

Figs. 4 and 5 show the relative sensitivity to uncertainty in the input parameters with respect to temperature. Note that we are able to preserve the spatial dimensions, allowing us to observe a given element's sensitivity to an input parameter with respect to the temperature at said point. Fig. 4 shows the mesh's sensitivity to fluctuations in the UO_2 pellets' power source-term. Not surprisingly we see that the temperature at the center of the basket is most sensitive to fluctuations in radioactive power. However, we should also note that the peak sensitivity is on the order of 0.3%, that is to say the total temperature expansions dependence on the power is only 0.3%.

Contrasted with the previous plot, we can see that the vast majority of the temperature expansion is accounted for by fluctuations in the actual boundary temperature. As we would expect the location that is 100% sensitive to the boundary wall temperature, is the boundary wall.

Acknowledgment

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