Anisotropic Azimuthal Power and Temperature Distribution Impact on Hydride Distribution

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INTRODUCTION

The extreme environment in which nuclear fuel operates provided a need for improved fuel analysis. The fuel simulation code BISON has been created at Idaho National Lab to address this need. BISON is a three-dimensional finite element based fuel performance code that can model temperatures, fission product swelling, densification, thermal and irradiation creep, fracture and fission gas production [1]. Of high importance in fuel performance is the degradation of the zirconium cladding. In the high temperature environment of a reactor, the zirconium in the cladding tends to corrode, and in the process hydrogen is released. Some of this hydrogen is absorbed by the cladding in a highly inhomogeneous manner. The distribution of the absorbed hydrogen is extremely sensitive to temperature, stress and concentration gradients. The absorbed hydrogen tends to concentrate near lower temperatures. This hydrogen absorption and hydride formation can cause cladding failure. This project set out to increase the hydrogen distribution prediction capabilities of the BISONcode. The project was split into two primary sections, first was the use of a high fidelity multi-physics coupling to accurately predict temperature gradients as a function of r, θ, and z, and the second was to use experimental data to create an analytical hydrogen precipitation model.

WORK PERFOMED

Multi-Physics Coupling

To obtain this hydrogen distribution accurately, it was necessary to calculate the three-dimensional temperature distribution in the cladding with a very fine resolution. To obtain such a distribution, it was decided to create a high fidelity multi-physics coupling. The coupling employed was a combination of DeCART and COBRA-TF (CTF). DeCART (Deterministic Core Analysis based on Ray Tracing) is a whole core neutron transport code for PWRs and BWRs. CTF (Coolant Boiling in Rod Arrays-Two Fluid) is a Penn State maintained multi-dimensional subchannel thermal hydraulics code. The codes were coupled using an independent Python script that ranDeCART and CTF inputs and passed information between the codes. The script passes local power information from the DeCART output to the CTF input. CTF then runs using this power distribution and passes local fuel temperature, bulk temperatures and bulk densities from CTF output to a new DeCART input. This process continued in an iterative fashion until a predetermined convergence criteria was met. The convergence was based on the difference in code calculated temperatures between each iteration. This code coupling is capable of running simulations for multiple depletion steps, thus it is able to simulate the entire lifecycle of a fuel load. Bison is a finite element based code, and thus the coupling between BISON-CTF and BISON-DeCART cannot be one to one. Additionally, BISON is only capable of modeling one pin at a time. Thus, the information from the DeCART-CTF coupling was stored as output files that were then fed into the BISON code. [2] See Figure 1 for a project overview.

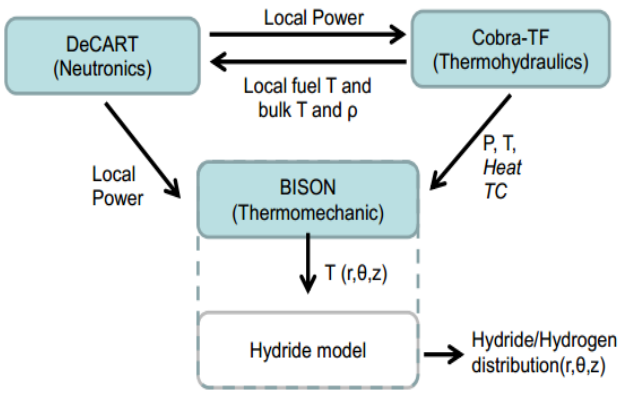

Fig. 1: Process outline flowchart [2]

Hydrogen Model

To accomplish this project, a hydrogen model kernel was created and implemented in the BISON code. A mean-field hydrogen model was used and the hydride distribution was considered at a mesoscopic scale. Theapproach for this model deals with basic principles of thermodynamics, material structure, and chemistry, using continuum models rather than an atomistic approach. To approximate the hydrogen distribution it is important consider diffusion, dissolution and precipitation. The precipitation of hydrogen in zirconium is mainly related to the terminal solid solubility (TSS). This TSS follows an Arrhenius law and is different for hydride precipitation and dissolution. [3,4]. Two diffusion mechanisms occur in the cladding: diffusion driven by concentration gradient and diffusion driven by temperature gradient. The diffusion gradient is governed by Fick's law, where thetemperature gradient is governed by the Soret effect. The diffusion flux is thus given by[5]:

$$J_{Fick} = -D\nabla C \tag{1}$$

$$J_{Soret} = -\frac{DCQ^*}{RT^2}\nabla T \tag{2}$$

The kinetics of precipitation and dissolution are given by [6 and 7]:

$$\frac{dC_p}{dt} = \alpha^2(C_{ss} - TSSp) \tag{3}$$

$$\frac{dC_{ss}}{dt} = -\alpha^2(C_{ss} - TSSp) \tag{4}$$

The heat of transport (Q*) and the precipitation rate constant (α^2) were determined experimentally.

The terminal solid solubility was determined by McMinn given by [8]:

$$TSSp\ (wt.ppm) = 138746.0 * exp\left(-\frac{4145.72}{T\ (K)}\right) \tag{5}$$

Experimental Determination of Precipitation Rate Constant α^2

The precipitation rate constant was found using the Advanced Photon Source at Argonne National Laboratory. The purpose of this experiment was to calculate the precipitation rate constant, α^2, by dissolving all hydrides in a charged zirconium cladding sample then cooling the sample rapidly and maintaining the sample temperature at various annealing temperatures to observe the hydride kinetics. A high intensity x-ray beam was used to produce diffraction patterns which allow for the intensity of the hydrides to be measured. This was done by integrating the diffraction patterns across the azimuth to obtain bulk concentration of hydrides in the form of hydride intensities. The experiment layout is shown in Figure 2. The precipitation rate constant is needed in order to analytically predict the concentration of hydrogen in solid solution.

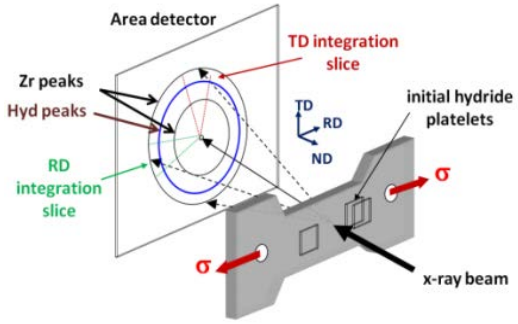

Fig. 2: Schematic of Precipitation Rate Constant experiment [9]

RESULTS

Water Rod Model

The test model created to run through the coupled codes was a four by four UO_2 pin array under standard PWR conditions. The layout is shown in Figure 3.

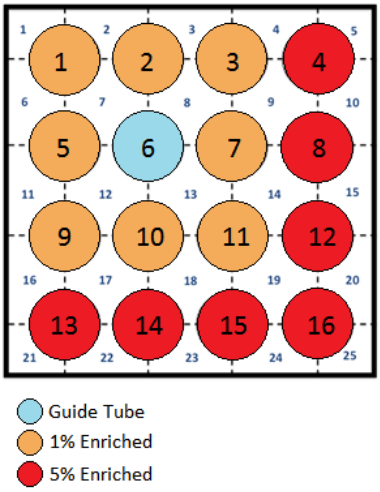

Fig.3: Core Model Layout

This first model was implemented as a test with the purpose of creating a large azimuthal temperature gradient at rod 11. The temperature and power distributions across pin 11 were calculated in the coupled code and inputted into the BISON program and hydrogen kernel with the results as shown in Figure 4 and 5 (both illustrations are rotated ninety degrees counter clockwise from the orientation depicted above). The results shown are for equilibrium conditions at the zero burnup step at the vertical center of the core.

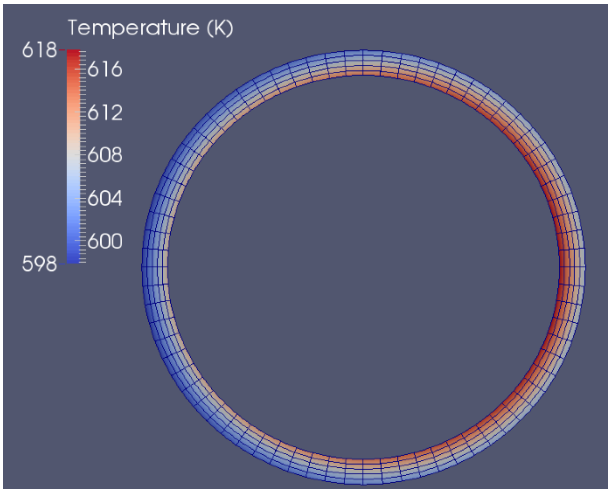

Fig. 4: Water rod model, rod 11 cladding temperature distribution

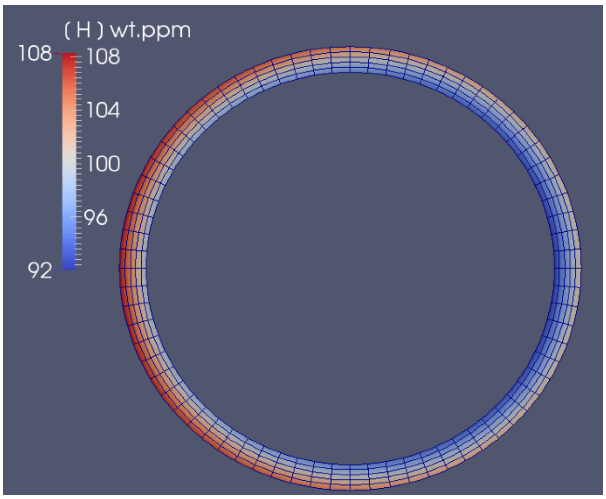

Fig.5: Water rod model, rod 11 cladding Hydrogen distribution

Spalled Oxide Model

A spalled oxide event occurs when a piece of ZrO_2 oxidation breaks away from the cladding causing an azimuthal variation in heat transfer. This was modeled in BISON by changing the heat transfer coefficient of one of the azimuthal sections of the cladding. The purpose of this simulation is to produce a large local temperature gradient for the hydrogen to act on. The simulation was run for 3 years with an initial hydrogen concentration of 50 wt.ppm. The temperature distribution and hydrogen concentration for this simulation can be found in Figures 6 and 7 respectively.

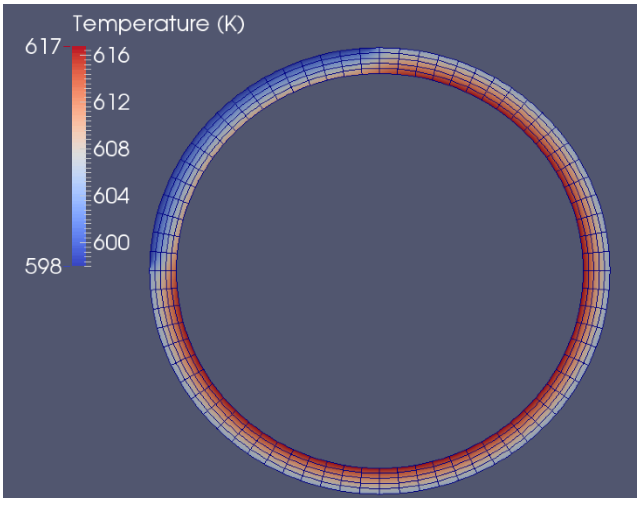

Fig6: Water rod model, rod 11 cladding Hydrogen distribution

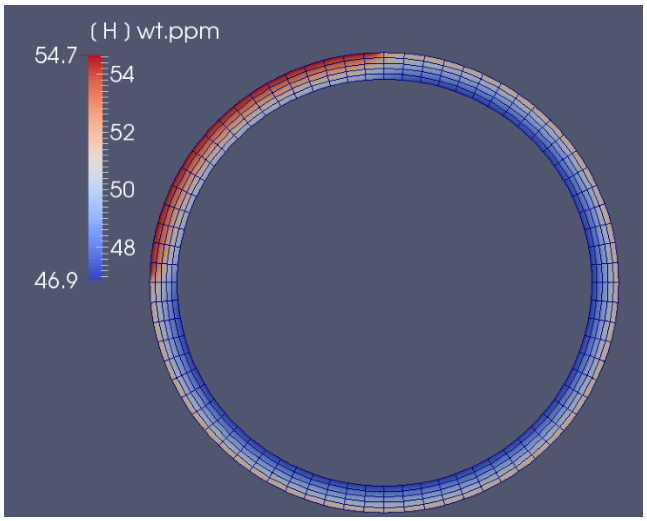

Fig7: Water rod model, rod 11 cladding Hydrogen distribution

Future Work

Future work includes the creation of several additional models. This includes the simulation of a control rod in place of the guide tube. This simulation and the water rod simulation will also be run for several depletion steps, in order to imitate a full fuel cycle. An additional model will use varying heat transfer coefficients in order to create an artificial boiling on one side of a pin. Additionally, the University of Michigan code coupling between CTF and neutronics code MPACT will be used to verify the results from the coupling described in this document.

NOMENCLATURE

α^2 = precipitation rate constant
ρ = Density
θ = aximuthal direction
C = Concentration
C_p = Amount of hydrogen in precipitated hydrides
C_{ss}= Amount of hydrogen in solid solution
J is the diffusion flux
N = concentration of hydrogen in solid solution
P = Power
Q* = heat of transport (according to Soret effect)
r = Radial direction
R = gas constant
T = Temperature
z = axial direction

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