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INTRODUCTION

Yttrium hydride (YH_x) is the main candidate for moderation of high temperature nuclear microreactors [1]. This is due to its high thermal stability and relatively high hydrogen retention at temperatures exceeding $870°C$. One of the main issues associated with the use of YH_x is that, when exposed to temperature, stress, or concentration gradients, the hydrogen contained in the metallic matrix tends to redistribute and leak from the moderating elements, potentially leading to reactivity losses and power swings. Recent attempts have been made to quantify this hydrogen redistribution feedback in realistic YH-moderated heat-pipe cooled microreactors. In Ref. [2], the hydrogen redistribution feedback was estimated for a unit-cell of a TRi-structural ISOtropic particles (TRISO)-fuelled heat-pipe-cooled microreactor by inputting realistic hydrogen concentration spatial distributions generated with the Stoichiometry With Internally Fluctuating Temperature (SWIFT) code in Griffin. The analysis in Ref. [2] has three main limitations: (1) SWIFT and Griffin were not coupled due to problems with licensing SWIFT outside of Los Alamos National Laboratory [1], and (2) the physical causes determining the reactivity coefficients were not discussed, and (3) it was performed on a unit-cell rather than at the full core level. In Ref. [3], Bison and Griffin were used in a coupled fashion to estimate the hydrogen redistribution feedback for the empire reactor unit-cell. While addressing the first two shortcomings of the analysis in Ref. [2], the results were still obtained for a unit-cell.

This paper is focused on presenting selected results from the asymptotic hydrogen redistribution analysis performed on the Simplified Microreactor Benchmark Assessment (SiMBA) problem, a microreactor core conceptual design developed at INL [4]. The analysis presented here overcomes the main limitations of Refs. [2, 3] since it is based on full core analysis, relies uniquely on Bison to perform hydrogen redistribution calculations, and discusses the physical causes of the reactivity feedback by developing preliminary observations performed at the unit-cell level in Ref. [3]. It was found that the feedback is negative, but it is one order of magnitude lower than the one found for the empire reactor unit-cell. This is due to the lower axial temperature gradient together with the effect of the reflector.

THEORY

Hydrogen Redistribution

Three driving forces lead to the redistribution of hydrogen in the YH_x bulk: (1) Fickian diffusion, redistributing hydrogen from regions of high concentration to regions of low concentration, (2) thermal diffusion (the Soret effect), redistributing the hydrogen from higher temperature zones to lower temperature zones, and (3) the stress gradients redistributing the hydrogen from high compression to high tensile regions. Since the stress-induced diffusion can be usually neglected due to its lower order of magnitude compared to Fickian and Soret diffusion [5], the hydrogen redistribution can be translated mathematically into the following equation [6]:

$$\frac{\partial c_H}{\partial t} = \nabla \cdot \left[-D \left(\nabla c_H + \frac{Q c_H}{RT^2} \nabla T \right) \right], \tag{1}$$

where c_H denotes the hydrogen molar concentration, D is the diffusion coefficient of hydrogen in Y_x, R the gas constant, T the temperature, Q is the heat of transport. For YH_x, the diffusion coefficient can be described by the following Arrhenius law [1]:

$$D = 10^{-8} \times \exp\left(\frac{-0.38[eV]}{RT} \right) \quad [m^2/s], \tag{2}$$

while the heat of transport $Q = 5300\, J/mol$ is constant with respect to hydrogen content and temperature. However, the heat of transport is unknown for YH_x. In absence of a better experimental results, the heat of transport for zirconium hydride is used due to the similarities. Please see Ref. [7] for a justification.

Heat Transfer

The heat conduction is modeled using the standard heat equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot \lambda \nabla T + S, \tag{3}$$

where, ρ and c_p denote the mass density and the specific heat, respectively, λ is the thermal conductivity, and S is the power density determined by the neutronic solver. The heat pipes are modeled through a Robin boundary condition:

$$\boldsymbol{J}_q \cdot \hat{n} = h\,(T - T_\infty)\,. \tag{4}$$

In Eq. 4, $h = 370 W/m^2/K$ denotes the heat transfer coefficient, $T_\infty = 900K$ is the temperature of the coolant of the secondary side (i.e., cooling the condenser region of the heat pipe). The value of the heat transfer coefficient was obtained by averaging Sockeye-computed heat transfer coefficient computed for the single heat pipes (the results are not shown in this paper).

Neutron Transport

The Discontinuous Finite Element- discrete ordinates (DFEM-SN) eigenvalue equations are used to model the neutron transport in the core. The equations can be expressed in operator notation as:

$$\mathcal{L}\boldsymbol{\psi} = \mathcal{S}\boldsymbol{\psi} + \frac{1}{k}\mathcal{F}\boldsymbol{\phi} - \mathcal{R}\boldsymbol{\psi}, \tag{5}$$

where $\boldsymbol{\psi} = \{\psi_{g,n}\}_{g=1,\dots,G;n=1,\dots,N}$ is the vector of angular fluxes for energy group g and along direction Ω_n. $\boldsymbol{\phi}$ is the vector of scalar fluxes, $\mathcal{L}$ contains streaming and collision contributions as well as the inter-element jump and vacuum boundary condition terms, $\mathcal{R}$ denotes the contributions from reflecting boundary conditions, $\mathcal{S}$ is the scattering operator, $\mathcal{F}$ is the fission operator and k is the multiplication factor. For a detailed description of the different operators, check the Griffin's user manual [8]. The DFEM-SN solver was chosen for its void compatibility and the scalability of the sweeper. The Coarse Mesh Finite Difference (CMFD) acceleration, recently implemented in Griffin was used to accelerate the problem convergence [9].

NUMERICAL RESULTS AND ANALYSIS

Problem Description

The Simplified Microreactor Benchmark Assessment (SiMBA) problem is an computational assessment problem based upon the empire reactor [10], the TRISO-fuelled concept in Ref. [2], and open eVinci^{TM} specifications [11]. The design details were chosen to be generic enough to avoid any proprietary concerns, while specific enough to capture the primary design characteristics of envisioned heat pipe-cooled monolithic microreactors. The SiMBA problem is a 2-MW microreactor composed of 18 hexagonal assemblies. Each assembly is composed of a UN-fueled 180-cm high active axial zone surrounded by 20-cm axial reflectors. Each assembly contains 96 fuel pins with 1-cm diameter, 60 YH pins with diameter of 0.975-cm, and 61 1-cm diameter heat pipes drilled into a graphite monolith. The heat pipes penetrate only into the top axial reflector, therefore making the power distribution axially asymmetric. This was done to obtain a net negative temperature reactivity coefficient The central shutdown rod slot is empty. The core is surrounded by 12 control drums and the reflector is hexagonal for a simplified mesh. Full geometric and material specifications are provided in Ref. [4] and are not reported in this article for the sake of brevity.

Codes and Computational Environment

DireWolf is a collection of codes built upon the Multiphysics Object-Oriented Simulation Environment (MOOSE) including Bison, Griffin, and Sockeye. A brief overview of Bison and Griffin, that were used to obtain the numerical results in this paper, are reported together with a description of Serpent. The latter code was used to generate macroscopic cross sections for the Griffin model. The interested reader is referred to the references in each subsection for in-depth codes' capabilities descriptions.

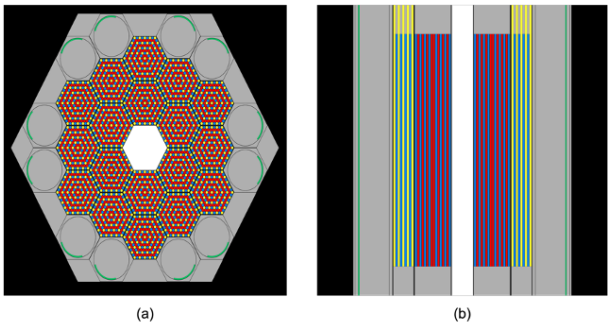

Fig. 1. (a) Radial view and (b) axial view of the Serpent model of the SiMBA problem.

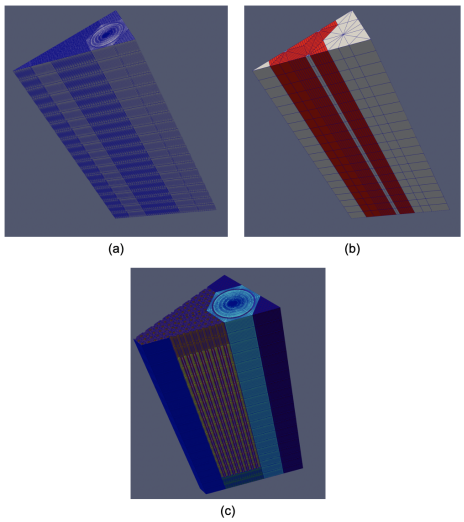

Fig. 2. Meshes for the (a) DFEM-SN, (b) CMFD, and (c) Bison models.

- Serpent 2 (V 2.1.32) is a continuous-energy Monte Carlo particle transport code developed at the VTT Technical Research Centre of Finland [12]. A Serpent model of the SiMBA problem was used to compute the multigroup cross sections using a 11-groups energy structure taken from Ref. [10]. The ENDF-VIII.0 library was utilized to capture the effect of $S(\alpha,\beta)$ libraries in yttrium hydride [13]. The cross sections are parametrized in terms of fuel temperature, $T_f(\boldsymbol{x})$, moderator temperature, $T_m(\boldsymbol{x})$, reflector temperature, $T_r(\boldsymbol{x})$, and stoichiometric ratio, HY. The variables are sampled using a Cartesian regular grid. The stoichiometric ratio is sampled using 0.1-spaced points in $HY \in [1.5, 2.0]$. Multigroup cross sections between state-points are computed by linear interpolation. A discussion on the parametrization of the cross sections with respect to hydrogen redistribution is object of ongoing work and will be reported in future work.

- Griffin is a MOOSE-based neutronics code designed to solve the neutron transport equation and its approximation. As mentioned in the theory section, the DFEM-SN solver accelerated with CMFD is used to compute the eigenvalue and the corresponding fission source spatial

distribution. For this exercise, 2 polar angles and 6 azimuthal angles per octant (i.e., 96 angles) are used for the simulation. The meshes for the DFEM-SN and CMFD models are shown in Figs. 2.a–b, respectively.

- Bison is a MOOSE-based nuclear fuel performance code able to solve the coupled equations of thermomechanics and species diffusion. In this paper, it was utilized to solve the heat diffusion equation coupled with the hydrogen redistribution equation. The mesh for the Bison model is shown in Fig. 2.c, respectively.

Multiphysics coupling is performed through Picard iteration, where the power density spatial profile computed with the DFEM-SN solver, here denoted as P, is provided to Bison, from which the corresponding fuel, moderator temperature profile, reflector temperature, and hydrogen distribution are obtained. The cross sections are then updated based on the value of temperature and stoichiometric ratio, which are provided to Griffin before an updated power profile is obtained. Iterations are performed until the L-2 relative residual norm between the initial and latest iterations falls below a specified tolerance. A representation of the calculation scheme is provided in Fig. 3.

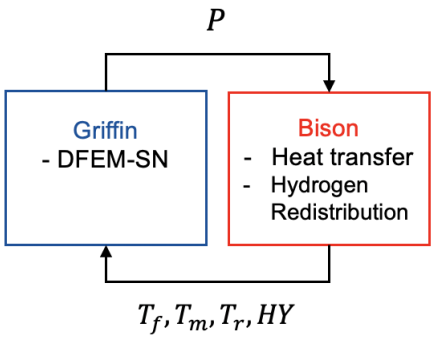

Fig. 3. Picard iteration scheme between Griffin and Bison.

Hydrogen Asymptotic Redistribution Reactivity Feedback

The hydrogen asymptotic redistribution feedback (HRF) is defined as the difference in multiplication factor, here denoted as k, between the system configuration characterized by flat hydrogen stoichiometric ratio, HY_0, and the one characterized by asymptotic hydrogen spatial distribution, HY_∞:

$$HRF = \frac{(k(HY_\infty) - k(HY_0))}{k(HY_0)}, \tag{6}$$

where the total quantity of hydrogen is conserved, *i.e.*,

$$\int_V C_\infty d^3x = \int_V C_0 d^3x. \tag{7}$$

In Eq. 7, C_0 and C_∞ denote the hydrogen concentration corresponding to the flat stoichiometric ratio HY_0 and the asymptotic stoichiometric ratio distribution HY_∞, respectively. For the SiMBA problem, the HFR is -50 pcm, with the multiplication factor passing from 1.27311 to 1.27264. As explained in Ref. [3], the negativity of the reactivity feedback is caused by the hydrogen migration towards axial zones characterized by lower moderator temperature. These zones are generally associated to lower neutron importance. Figure 1.b–1.c shows the 3D moderator temperature distribution and the corresponding HY_∞ distribution. It is noticeable that the zones characterized by high stoichiometric ratio, HY, corresponds to the zones characterized by low T_m, consistently with Eq. 1 and the results found in Ref. [3].

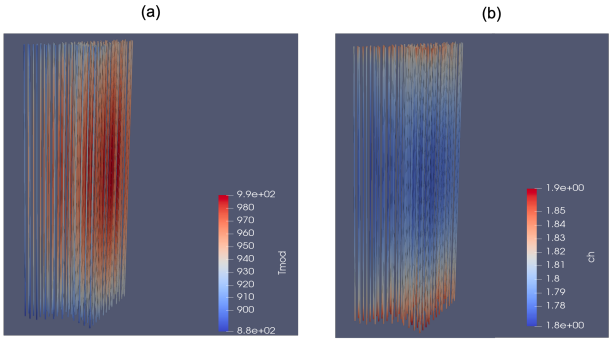

Fig. 4. (a) Moderator temperature and (b) hydrogen spatial distributions.

However the HFR found on the full-core is ten times lower than the one computed for the empire unit-cell in Ref. [3]. This is due to two reasons. The first one is that the axial moderator temperature gradient is much lower than the one found for the empire unit-cell. This is evident from Fig. 5, where the radially-averaged moderator temperature is plotted for 20 10-cm high axial layers. The radially-averaged moderator temperature varies between 900 K and 931 K, determining a max-min difference of 30 K. This is much lower than the one computed for the empire unit-cell (*i.e., 100 K*), determining a milder redistribution of hydrogen. In fact, maximum and minimum stoichiometric ratio for the SiMBA problem are 1.860 and 1.765, respectively. This is in contrast to a maximum-minimum stoichiometric ratio difference of 0.5 in the empire reactor unit-cell.

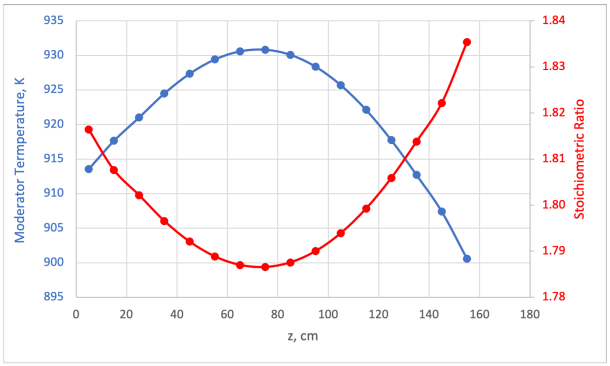

Fig. 5. Radially-averaged moderator temperature and stoichiometric ratio axial profiles.

The second factor affecting the magnitude of the coefficient is the presence of 20-cm beryllium reflectors. In fact, the neutron scattered back from the reflector generate power peaks, that can be considered proxies to neutron importance peaks,

near the axial periphery of the reactor. Yet, these axial zones are associated to lower moderator temperatures, therefore determining a local migration of hydrogen towards higher importance zones, in contrast to the general trend. This is graphically visible in Fig. 6, where the radially-averaged power distribution and the radially-averaged stoichiometric ratio are plotted against the axial coordinate (with origin at the beginning of the active axial zone). This reflector-driven effect was negligible in the unit-cell modeled in Ref. [3], where the reflector was just 1-cm thick, therefore mitigating the power peaks. It is also important to notice that the power profile is not strongly affected by the hydrogen migration (data not shown). In fact, the maximum power variation happens in the closest point to the top reflector where the hydrogen change reaches its maximum value (radially-integrated power changes of 5.2% between flat and asymptotic *HY* distribution).

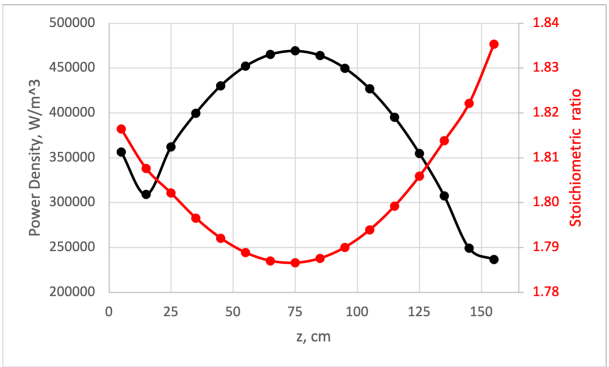

Fig. 6. Radially-averaged power density and stoichiometric ratio axial profiles.

CONCLUSIONS AND FUTURE WORK

In this paper, selected results from the asymptotic hydrogen redistribution analysis performed on the SiMBA reactor problem were presented. This analysis was performed to overcome the main limitations of previous works on the subject for heat-pipe cooled YH-moderated microreactor [2, 3]. It was found that the asymptotic HRF was -50 pcm. The sign of the feedback is the same as the ones in Refs. [2, 3]. However, the order of magnitude of the feedback was lower than the one found for the empire reactor unit-cell. The difference stems from two reasons. First, the moderator temperature axial gradient is much lower than the one seen for the empire unit-cell. Second, the presence of a 20-cm beryllium reflector creates power peaks at the axial periphery. Since these are zones in which the moderator temperature reaches its minimum value, local migration of hydrogen into higher importance zones occurs, therefore lowering the absolute value of the total negative HRF of the reactor. Future work will be devoted to exploring two main research avenues. The first will consist in incorporating the thermomechnic response of the system. The second one is to extend the analysis to transient scenarios. To perform this task, current work is being devoted to including the heat pipes transient response and the hydrogen leakage model described in Ref. [1].

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