One-Dimensional Neutronic Analysis of BWR Hydride Fuel Bundles

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Abstract

An approximate, yet useful methodology to simulate the neutronics of BWR fuel bundles using a series of 1-D unit cell calculations was developed using the code sequence SAS2H of the SCALE-5 code package. Based on experimentation with a number of different bundle axial power distributions and of different number of axial zones the bundle is divided into, it is concluded that the preferred approach for predicting the BWR k_∞ evolution and discharge burn-up is to consider the entire enriched fuel region as a single zone having the average region power density and water density. This procedure was then applied to construct two-dimensional maps of attainable discharge burn-ups for BWR cores as a function of the BWR clad outer diameter and pitch-to-diameter ratio. It was also found that SAS2H can adequately account for the bound hydrogen scattering kernel of zirconium hydride.

KEYWORDS: hydride fuel, BWR, unit-cell analysis, burn-up, SAS2H

1. Introduction

The feasibility of improving the performance of BWR cores by designing them to operate on hydride rather than oxide fuel has been under investigation as part of NERI project 02-189 [1-3]. The general objective of the present study is to determine the attainable discharge burn-up from BWR cores fueled with U-$ZrH_{1.6}$ fuel for a large combination of fuel rod outer diameter (D) and lattice pitch (P) while meeting by the constraints of sufficiently negative fuel temperature reactivity coefficients as well as negative reactivity effect due to coolant voiding.

Oxide fuelled BWR fuel bundles are characterized by a large non-uniformity in both radial and axial directions due to (a) the inclusion of water rods, partial length fuel rods and wide water gaps between bundle boxes in addition to use of a large number of uranium enrichment levels; (b) large axial variation in the water density.

In order to accurately account for these non-uniformities, we used the MOCUP (MCNP5 + ORIGEN 2) code system [4] for a detailed 3-D fuel bundle analysis [3]. However, MOCUP is prohibitively time consuming for a scoping study that has to span a large D-P design space. On the other hand, 1-D unit cell depletion analysis is not straightforward to apply to BWR, as to PWR cores, due to the large axial variation of the water density and heterogeneity of the BWR fuel bundles. A specific objective of this work is to develop an approximate, yet useful methodology to simulate the neutronics of BWR fuel bundles using the 1-D unit cell codes sequence SAS2H of the SCALE-5 code package [5].

2. Benchmarking hydride fuelled unit cell

Before applying SAS2H for the BWR parametric study, it was benchmarked against MOCUP for simulating a representative hydride fuelled single pin unit cell. Previous benchmarks made between SAS2H and MOCUP, considering oxide and MOX fuel and water moderator showed good agreement [6]. In order to amplify the effects of the zirconium hydride, that is the novel constituent of the hydride fuel, in the benchmark $ZrH_{1.6}$ was chosen as moderator instead of water.

A Wigner-Seitz cylindrized cell with an isotropic reflection on the radial boundary and an optical reflection on the axial one was used for the analysis. The power is assumed to be 58.24 kW. The benchmark unit cell geometry and materials density are summarized in Tables 1, 2 and 3.

Table 1: Benchmark unit cell geometry

Fuel rod radius [cm]	0.52197
Clad inside radius [cm]	0.53213
Clad outside radius [cm]	0.61341
Pitch [cm]	1.6256
Height [cm]	370.84

Table 2: Characteristics of U(45w/o)$ZrH_{1.6}$ fuel with 5 % enriched U

Isotope	Atomic density (atoms/b-cm)
^{235}U	7.607691e-04
^{238}U	1.427203e-02
H	2.405248e-02
Zr	1.503280e-02
Temperature	800 K

Table 3: $ZrH_{1.6}$ moderator characteristics

Isotope	Atomic density [atoms/b-cm]
H	5.822568e-02
Zr	3.639105e-02
Temperature	800 K

Table 4 and Figures 2, 3 and 4 compare selected results obtained with SAS2H and MOCUP. It is found that the two codes are in good agreement in their calculated integral parameters such as k_∞ and in the time evolution of the important fuel isotopes.

Table 4: Infinite multiplication factor at BOL

Code	Scattering Kernel	$k_\infty \pm \sigma$	Difference SCALE-MCNP
MCNP	Applied	1.41829 ± 0.00009	-
SAS2H	Applied	1.40220	-1.141%
MCNP	Not applied	1.41891 ± 0.00009	-
SAS2H	Not applied	1.40464	-1.0107%

Figure 1: k_∞ as function of exposure time comparison

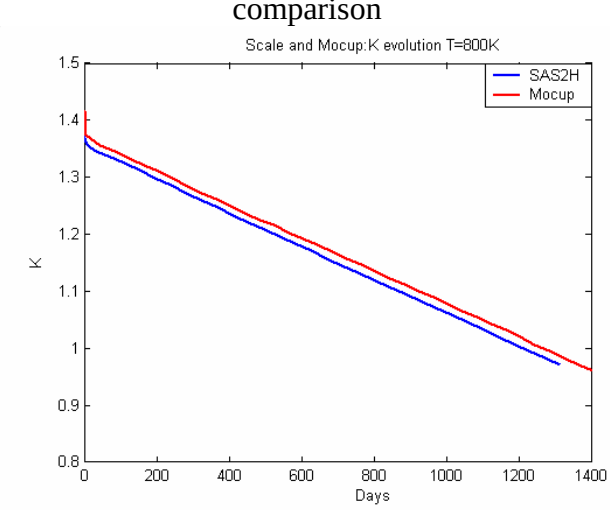


Figure 2: ^{235}U concentration as function of exposure time comparison

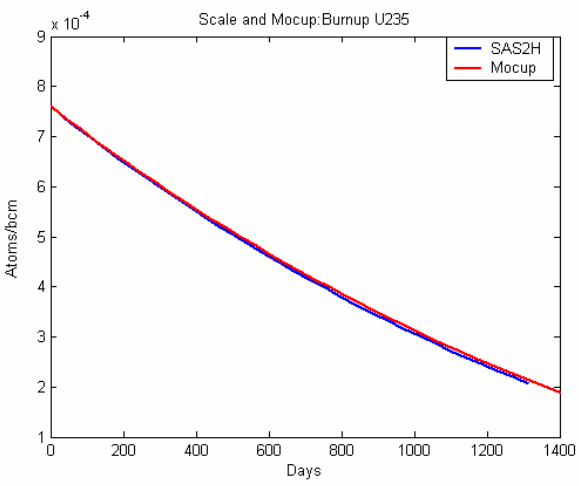


Figure 3: ^{238}U concentration as function of exposure time comparison

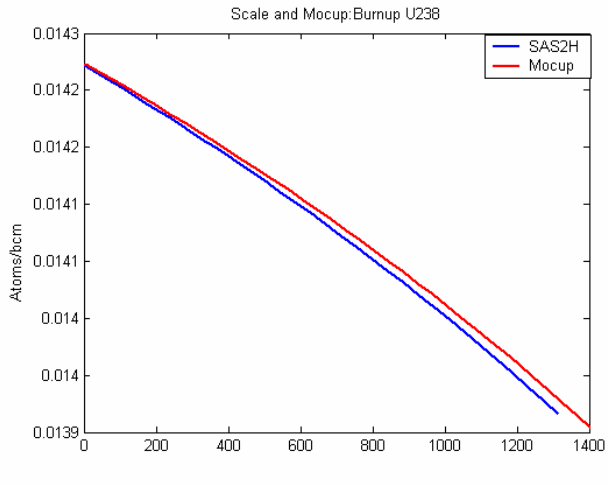
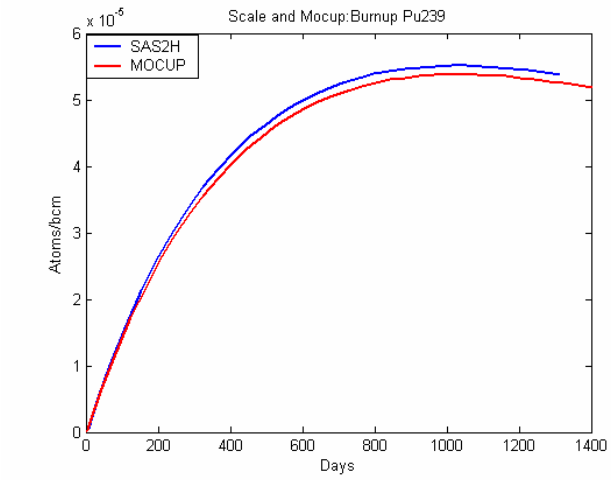


Figure 4: ^{239}Pu concentration as function of exposure time comparison



3. Methodology

The methodology developed for simulating a BWR fuel bundle neutronic characteristics using a sequence of 1-D unit cells analysis starts with geometric modeling approximations of the actual fuel bundle. The objective is to achieve a bundle-averaged neutron spectrum that well represents the fuel bundle and to obtain a good agreement with the 3-D results for the evolution, with burn-up, of k_∞ and of the inventory of the most important actinides.

The procedure developed involves dividing the fuel bundle into N axial zones. For each of these zones an effective unit cell is defined to have D and P as in the fuel bundle while the composition is determined using the following assumptions:

1) Water density

The water density to be used in the single pin model should provide the bundle average water-to-fuel mass ratio:

$$\left(\frac{M_{Water}}{M_{Fuel}}\right)_{Bundle} = \left(\frac{M_{Water}}{M_{Fuel}}\right)_{Pin} . \quad (1)$$

The above equality can be expressed as

$$\left(\frac{M_{Water}}{M_{Fuel}}\right)_{Bundle} = \frac{\bar{\rho}_W^B \cdot V_W^B}{\bar{\rho}_F^B \cdot V_F^B} = \frac{\bar{\rho}_W^B \cdot V_W^B}{\bar{\rho}_F^B \cdot N_{FR} \cdot V_F^P} = \left(\frac{M_{Water}}{M_{Fuel}}\right)_{Pin} = \frac{\rho_W^P \cdot V_W^P}{\rho_F^P \cdot V_F^P} \quad (2)$$

where $\bar{\rho}_W^B$ and ρ_W^P is the average water density in the bundle and in the single pin unit cell, $\bar{\rho}_F^B$ and ρ_F^P is the average fuel density in the bundle and in the unit cell while V_W^B and V_W^P is the water volume in the bundle and in the single pin unit cell. If V_{WR} is the volume of water in one water rod and V_{out} is the volume of water in the water gap surrounding the fuel bundle,

$$\rho_W^P = \bar{\rho}_W^B \cdot \left(\frac{N_{WR} \cdot V_{WR} + V_{out}}{N_{FR} \cdot V_W^P} + \frac{N_{WR}}{N_{FR}} + 1\right) \quad (3)$$

where it was assumed that $\rho_F^P = \bar{\rho}_F^B$.

2) Structural material

Likewise, the amount of structural material used in the unit cell should represent the total mass of zirconium in the fuel bundle, including the Zr of the external bundle box and in the clad of the water rods. This extra structural material is uniformly mixed with the water coolant of the unit cell. The expression used to account for the extra structural material is the following:

$$\rho_{ZR}^{Eq} = \left[\frac{\left(a^2 - b^2\right) \cdot H \cdot \rho_{ZR}^{BOX} + N_{WR} \cdot \pi \cdot \left(COR^2 - CIR^2\right) \cdot H \cdot \rho_{ZR}^{WR}}{N_{FR} \cdot V_{MOD}^{PIN}}\right] \quad (4)$$

where $V_{MOD}^{PIN} = \left[P^2 - \pi \cdot COR^2\right] \cdot H$,

a and b are the external and internal dimension of the bundle box,
COR and CIR are the clad outer and inner diameters,
H is the bundle length,
N_{FR} and N_{WR} are the number of fuel rods and of water rods per fuel bundle,
ρ_{ZR}^{BOX} is the density of the zirconium in the bundle box, and
ρ_{ZR}^{WR} is the density of the zirconium in the clad of the water rods

3) Enrichment of fissile material

Due to limitations in the geometric modelling capability of SAS2H, an explicit representation of the distributed pin enrichment is not possible. Instead, the bundle-average enrichment for each axial zone is used for the enrichment of the single pin.

4) Axial power distribution

A different power level is assigned to each zone corresponding to its axial position in the bundle. Two different axial power shapes were considered:
(a) The MCNP calculated axial power;
(b) Uniform power (unchanged throughout exposure).

If natural uranium pellets are located at the bottom and top of the fuel rods, the fractional power generated by these zones was calculated and kept constant throughout the cycle.

With these approximations, the following procedures were used to average the results of all the zones in order to get the average bundle parameters:

a) k_∞ averaging

The k_∞ for each zone i is calculated as:

$$k_{\infty,i} = \frac{\nu_i \int_{V_i} \Sigma_{f,i}\phi_i dV}{\int_{V_i} \Sigma_{a,i}\phi_i dV} \quad . \tag{5}$$

As zone i power is $P_i = E_f \int_{V_i} \Sigma_{f,i}\phi_i dV$, the bundle average k_∞ is:

$$k_\infty = \frac{\sum_i \nu_i \int_{V_i} \Sigma_{f,i}\phi_i dV}{\sum_i \int_{V_i} \Sigma_{a,i}\phi_i dV} = \frac{\sum_i \nu_i P_i}{\sum_i \frac{\int_{V_i} \Sigma_{a,i}\phi_i dV}{\int_{V_i} \Sigma_{f,i}\phi_i dV} P_i} = \frac{\sum_i \nu_i P_i}{\sum_i \frac{\nu_i P_i}{k_{\infty,i}}} \quad . \tag{6}$$

Assuming that ν_i is zone independent, Equation (6) becomes

$$\frac{P}{k_\infty} = \sum_i \frac{P_i}{k_{\infty,i}} \tag{7}$$

b) Actinides concentration averaging

The total concentration A_i of actinide i is:

$$A_i = \sum_{j=1,N} A_i^j \frac{V_j}{V^{TOT}} \tag{8}$$

where:

A_i^j is the concentration of actinide i in zone j

V_j is the volume of the j^{th} zone, and

N is the number of axial zones

4. Methodology validation

The above described procedure was tested against the results obtained using the 3-D MOCUP analysis for a couple of fuel bundle geometries and compositions.

The first is the reference 9x9 oxide fuel bundle described in detail in reference [3] that is very heterogeneous – it has 8 different types of fuel rod compositions, water rods, partial length fuel rods and relatively wide water channels around the bundle box. Natural uranium pellets are

located at the bottom and top of the fuel rods. The geometry and composition of this fuel bundle were accurately simulated with MOCUP using 24 depletion zones corresponding to the 24 enrichment zones. The fraction of the bundle power generated in each depletion zone was calculated by MOCUP at each burn-up step. The axial coolant density distribution was represented using 24 equal length axial zones. Gadolinium was not included in this analysis.

The second bundle simulated is the reference 10x10 hydride fuel bundle [3]. It is fuelled with TRIGA type U-$ZrH_{1.6}$ having 45 wt % U. The bundle pitch is the same as of the reference oxide bundle. Its 10x10 array of rods is contained in the same volume as occupied by the reference 9x9 oxide fuel bundle, including the water moderator volumes. Of its 100 rods, 96 are full length hydride fuel rods versus only ~71 effective full length fuel rods in the reference oxide fuel bundle. The remaining 4 sites house control rods guide tubes. Being of significantly more uniform design, only 9 depletion zones were considered in the MOCUP simulations for hydride fuel bundles – 3 equal length axial and 3 radial zones.

In order to apply the SAS2H methodology developed in the previous section, the fuel bundle was divided into either N=1 or 3 (the top and the bottom of natural uranium and one central zone) or 5 axial zones (two for the top and the bottom natural uranium zones and three equal length zones for the rest of the fuel). An effective unit cell is defined for each zone.

Figures 5 through 8 compare the evolution with burn-up of k_∞ as calculated using SAS2H versus MOCUP. Good agreement was obtained even when using a single axial zone (N=1). In the oxide case the agreement improves with the number of the axial zones used in the 1-D model. The relative error shown in Figure 6 and 8 is defined as

$$\frac{\Delta k}{\bar{k}} = 2\frac{k_{SCALE} - k_{MOCUP}}{k_{SCALE} + k_{MOCUP}} \tag{9}$$

Figure 5: Reference oxide fuel core average k_∞ as a function of operation time

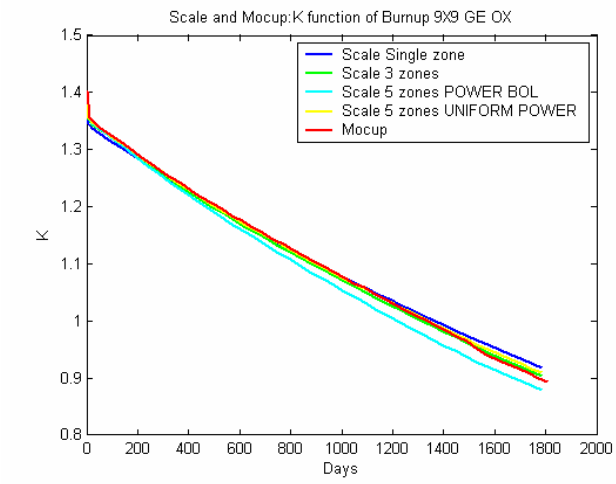


Figure 6: Relative error in k_∞ as a function of operation time

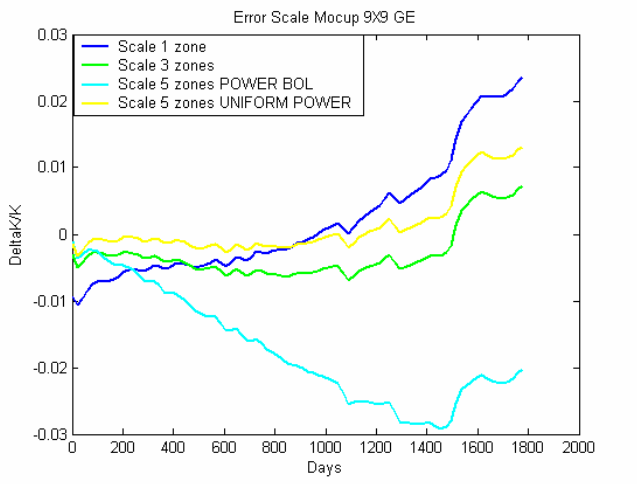


Figure 7: Reference hydride fuel core average k_∞ as a function of operation time

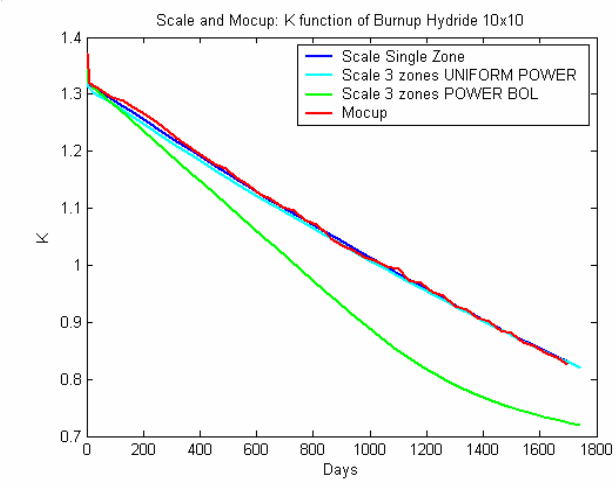
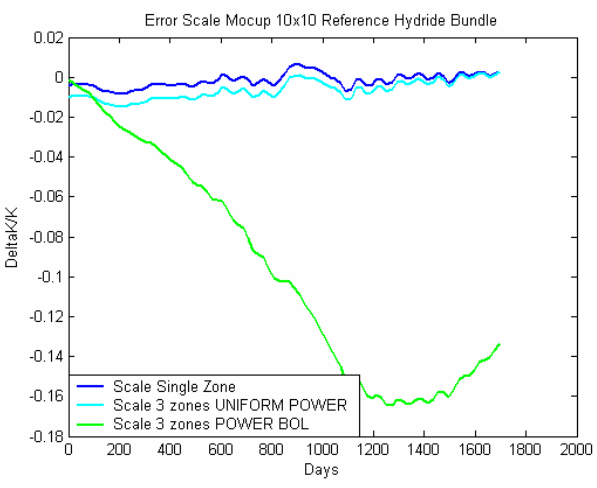


Figure 8: Relative error in k_∞ as a function of operation time



In the comparison against the oxide bundle, it is found that the single zone approach under-predicts k_∞ at BOL and over-predicts it after about 800 days. The 5-zone approach, using BOL axial power shape, under-predicts k_∞. The best SAS2H results in both comparisons were obtained assuming a uniform axial power distribution.

Based on these simulations it is concluded that the preferred approach for predicting the BWR k_∞ evolution and discharge burn-up, based on simple 1-D analysis, is to consider the entire enriched fuel region as a single zone having power density and water density equal to the average of the region. This approach was used to generate the BWR discharge burn-up maps.

5. BWR discharge burn-up maps

As a part of the NERI project, [1] discharge burn-up maps were generated with SAS2H for a 3-batch PWR core fuelled with U-$ZrH_{1.6}$ having 5% enriched uranium. A burn-up map is a 2-D design space where the design variables considered are the fuel rod outer clad diameter (D or COD) and the lattice pitch-to-diameter ratio (P/D). For every design point (COD, P/D) the discharge burn-up values were calculated without burnable poison and without soluble boron. The range of the design variables explored is: 0.65 cm ≤ COD ≤ 1.25 cm and 1.05 ≤ P/D ≤ 1.6. Figure 9 and 10 reproduce the attainable PWR burn-up maps. Figure 10 shows the achievable burnup constrained by the conditions that all the "core averaged" reactivity coefficients be always negative. These results do not account for the use of soluble boron, as is the case in BWR.

The BWR burn-up maps are derived from the above PWR burn-up maps using a correlation between $(COD, P/D)_{BWR}$ and $(COD, P/D)_{PWR}$. The correlation is based on the equality of the total hydrogen-to-heavy-metal atom ratio in the fuel bundles:

$$\left(\frac{H}{HM}\right)_{BWR} = \left(\frac{H}{HM}\right)_{PWR} \tag{10}$$

Writing it in explicit form and solving for $\left(\frac{P}{D}\right)_{PWR}$ after simplifications we get:

$$\left(\frac{P}{D}\right)_{PWR} = \sqrt{\frac{\rho_{H2O}^{BWR}}{\rho_{H2O}^{PWR}} \cdot \left(\frac{R_{FUEL}^{PWR}}{R_{FUEL}^{BWR}}\right)^2 \cdot \left(\frac{COD^{BWR}}{COD^{PWR}}\right)^2 \cdot \left(\frac{P}{D}\right)_{BWR}^2 + \frac{\pi}{4} \cdot \left[1 - \frac{\rho_{H2O}^{BWR}}{\rho_{H2O}^{PWR}} \cdot \left(\frac{R_{FUEL}^{PWR}}{R_{FUEL}^{BWR}}\right)^2 \cdot \left(\frac{COD^{BWR}}{COD^{PWR}}\right)^2\right]} \qquad (11)$$

Equation (11) correlates a given effective BWR unit cell with a PWR unit cell having the same fuel pellet diameter and the same H/HM ratio. The BWR and PWR unit cell pitch will, in general, be different.

This conversion methodology was found to give acceptable agreement in the k_∞ evolution with burn-up and in the BOL neutron spectrum as illustrated in Figures 11 and 12. Compared in these figures are the results from our 1-D model analysis for the equivalent PWR and BWR unit cells defined in Table 5.

Table 5: PWR reference geometry and BWR equivalent geometry

Reactor	PWR	BWR
Fuel rod diameter [cm]	1.0422	1.0422
Clad inside diameter [cm]	1.0727	1.0634
Clad outside diameter [cm]	1.2055	1.24205
P/D	1.277	1.3
Pitch [cm]	1.5398	1.6146

Figures 13 and 14 display the achievable burn-up maps for the effective 1-D BWR unit cells that were constructed from the PWR burn-up maps of Figures 9 and 10 using the above described conversion methodology.

Figure 9: PWR achievable burn-up [GWD/MTHM] map not accounting for reactivity constraints.

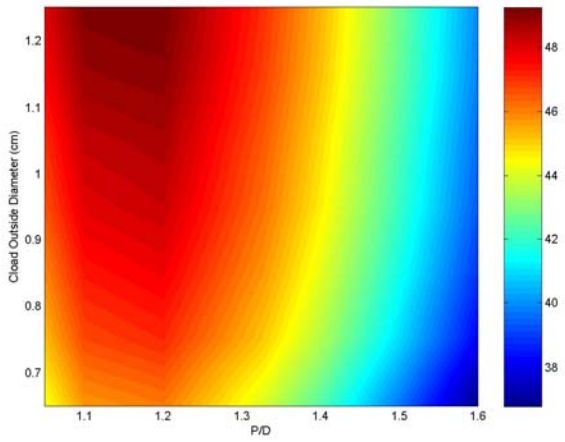


Figure 10: PWR achievable burn-up [GWD/MTHM] map accounting for reactivity constraints.

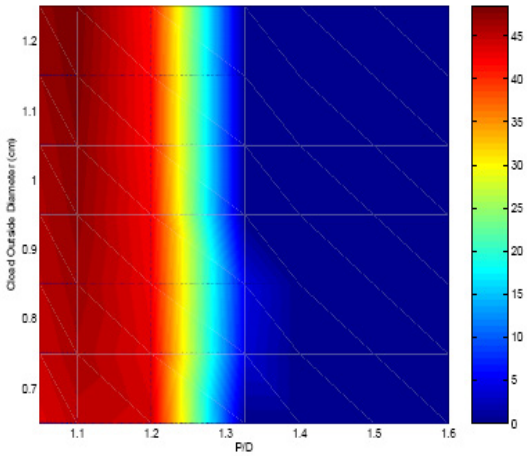


Figure 11: k_∞ as function of exposure time for the PWR reference geometry and the BWR equivalent geometry

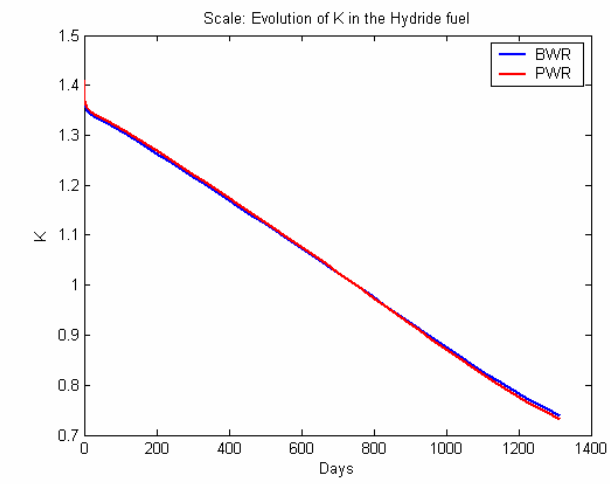


Figure 12: Neutron spectrum at BOL for the PWR reference geometry and the BWR equivalent geometry

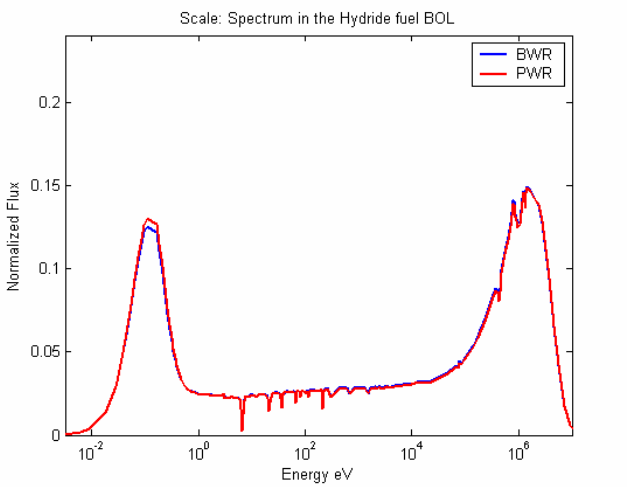


Figure 13: BWR achievable burn-up [GWD/MTHM] map not accounting for reactivity constraints

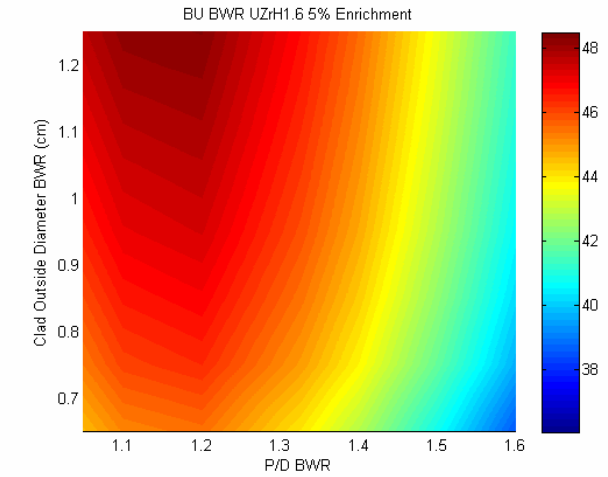
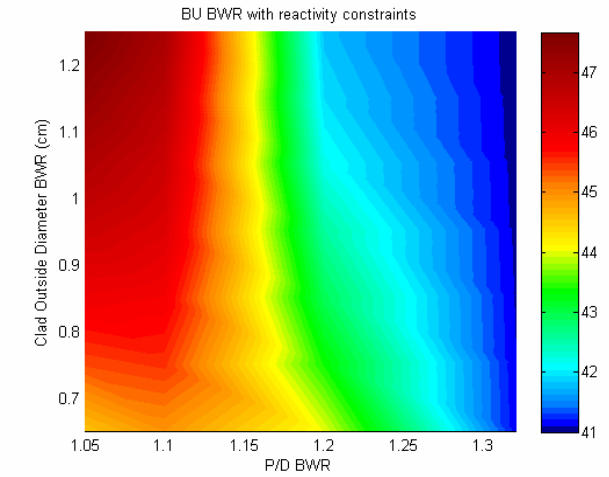


Figure 54: BWR achievable burn-up [GWD/MTHM] map accounting for reactivity constraints



6. Conclusions

An approximate, yet useful methodology to simulate the neutronics of BWR fuel bundles using a series of 1-D unit cell calculations was developed using the code sequence SAS2H of the SCALE-5 code package. The methodology involves dividing the BWR fuel bundle into N axial zones. For each of these zones an effective unit cell is defined to have the actual fuel diameter and an effective pitch. The effective pitch is defined so as to conserve the total amount of water and of structural material as in the fuel bundle. The structural material, excluding the fuel rod cladding, is uniformly distributed in the water. The single pin cell water density is the bundle average water density at the axial zone considered. An algorithm was developed to estimate the bundle average k_∞ and bundle total inventory of individual fuel isotopes based on a series of 1-D simulations of each of the bundle axial zones. Based on experimentation with a number of

different axial power distributions and different number of axial zones it is concluded that the preferred approach for predicting the BWR k_∞ evolution and discharge burn-up based on simple 1-D analysis is to consider the entire enriched fuel region as a single zone having the average region power density and water density. This procedure was then applied to construct two-dimensional maps of attainable discharge burn-ups for BWR cores from attainable burn-up maps that were available for PWR cores.

It was also found that SAS2H can adequately account for the bound hydrogen scattering kernel of zirconium hydride.

Acknowledgment

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