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Physics Characteristics of U-$ZrH_{1.6}$ Fueled PWR Cores

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This paper summarizes part of the neutronic studies performed for NERI project 02-189 aimed at assessing the feasibility of improving the performance of light water reactors by using solid hydride fuel instead of oxide fuel. Infinite lattice neutronic parametric study indicates that it should be possible to design PWR cores using U-$ZrH_{1.6}$ fuel to have comparable discharge burnup as attainable with UO_2 fuel of same enrichment. The optimal hydride fuel P/D ratio is significantly smaller than that of oxide fuel but has a softer spectrum. U-$ZrH_{1.6}$ fuelled cores can be designed to have negative coolant and fuel temperature coefficient of reactivity. U-$ZrH_{1.6}$ fuel offers a couple of unique temperature reactivity feedback mechanisms – a prompt feedback due to spectrum hardening and a delayed feedback due to hydrogen diffusion. Handling of hydride fuel will require special attention to criticality safety.

KEYWORDS: hydride fuel, U-$ZrH_{1.6}$, PWR, optimal P/D, burnup, reactivity coefficients, criticality safety

1. Introduction

This paper summarizes part of the neutronic studies performed so far under a NERI sponsored project. The objective of this project is to assess the feasibility of improving the performance of light water reactors by using solid hydride fuel instead of oxide fuel. Two general types of hydride fuel are considered in the NERI project: one based on zirconium hydride and the other based on thorium hydride. Either enriched uranium or plutonium is considered for the fissile material. Applications to both PWR and BWR are being considered. The neutronic analysis described in this paper considers U-$ZrH_{1.6}$ fuel in PWR.

Following a general review of hydride fuel properties and the incentives for considering it for LWR (Sec. 2), we describe the calculation approach used (Sec. 3) and summarize part of the results obtained so far (Sec. 4).

2. Hydride Fuel

2.1 Background

Uranium-zirconium hydride fuel has been in use in dozens of water-cooled TRIGA type research reactors for dozens of years. It has been developed for TRIGA reactors because of its unique safety characteristic – a prompt negative reactivity feedback due to spectrum hardening with fuel temperature increase. This feedback mechanism enables pulsing TRIGA reactors to very high peak powers. Uranium-zirconium-hydride fuel has also been used in at least one liquid metal cooled space nuclear power reactor that operated at significantly higher coolant temperatures than LWRs.

2.2 Properties

U-$ZrH_{1.6}$ fuel has been extensively studied, tested in reactors and has an impressive record of safety. The thermal conductivity of the TRIGA fuel is nearly 5 times larger than that of

UO_2. Consequently, the peak fuel temperature under typical LWR operating conditions is estimated to be below 700°C. This provides a large margin to accommodate transients that lead to fuel temperature increase even in LWR conditions that feature significantly higher water coolant temperature than the water temperature in TRIGA reactors.

TRIGA type fuel achieved a discharge burnup of approximately 100 GWd/tHM – just about twice that of LWR, without fuel rod failures or deformations exceeding functional limits. The fission gas fraction released from TRIGA fuel and from hydride fuel of space reactors is reported to be very low as compared with oxide fuel.

U-$ZrH_{1.6}$ fuel has relatively small uranium density – only about 40% of the uranium density in UO_2 fuel. However, the total U loading in an optimal hydride fuel core was found to be close to that of an oxide fuel core due to the larger fuel volume fraction in the hydride core. U-ThH_2 fuel features close to 20% higher heavy metal inventory than equal volume UO_2 fuel.

A possible drawback of hydride fuels is that they are not compatible with Zircaloy cladding. However, there appear to be practical solutions to this problem. One possible solution is to form hydrogen impermeation barrier on the inner Zircaloy clad surface; oxide layer or a thin liner of appropriate material (such as Al or Be) might provide such a barrier. A last resort solution is to use stainless-steel cladding.

2.3 Incentives for using Hydride Fuel in LWR

The hydrogen concentration in U-$ZrH_{1.6}$ fuel is comparable to that of water at PWR operating conditions (~0.7 g/cm^3). The introduction of part of the hydrogen needed for neutron moderation within the fuel volume permits attainment of optimal neutron spectrum without increasing the core volume. Increasing the moderation ratio could enable higher discharge burnup and recycling plutonium more effectively in LWR. With hydrogen in the fuel, the lattice pitch can be smaller and larger number of fuel rods can be loaded into a core of a given volume. The result could be a higher power level from the same core volume.

Moreover, thorium hydride fuel has a higher heavy metal (HM) density than oxide fuel. As a result U-ThH_2 or Pu-ThH_2 fueled cores can be designed to have a significantly longer core life and higher energy generation per core loading than achievable with the corresponding oxide fueled cores. The net outcome is expected to be improved economics, improved resource utilization, reduced waste, improved proliferation resistance and improved safety.

Hydride fuel can also replace water rods and/or moderator volumes in BWR and SCWR cores and thus further increase the number of fuel rods and power output of a given volume core. The resulting fuel assembly design is significantly less heterogeneous.

In addition to the unique prompt reactivity feedback (Sec. 2.1), hydride fuel offers a unique delayed negative reactivity feedback mechanism – spectrum hardening due to some hydrogen dissociation from the metal hydride and migration to the fission gas plenum. This dissociation will not affect the hydride fuel integrity; it is a reversible process.

The prompt feedback mechanism could enable loading plutonium and, possibly also minor actinides in LWRs using uranium-free fuel, thus improving the Pu (MA) incineration capability of LWRs.

3. Methodology

3.1 Approach

The neutronic analysis is based on parametric studies of infinite unit cells. The variable parameters of the unit cell are the fuel rod diameter, the lattice pitch, the fuel type – hydride or oxide, and the uranium enrichment. The burnup analysis done corresponds to a single batch fuel management scheme. The discharge burnup is assumed to be that burnup for which k_∞ is

1.03. An estimate of the discharge burnup attainable in a 3-batch fuel management can be obtained by increasing the single-batch burnup value by 50%.

3.2 Computational Methods

Most of the calculations are performed with the WIMSD-5B code and its associated cross-section library [1]. This code was first benchmarked against MCNP4B2 [2] and SCALE4.4 SAS2H sequence [3]. MCNP and SCALE calculations take into account the effect of hydrogen binding in the zirconium hydride lattice on neutron scattering. The WIMS code uses the free hydrogen scattering kernel.

Table 1 defines the reference uranium oxide and hydride fuel unit cells considered for the benchmark. The Zircaloy-4 density is assumed to be 6.56 g/cm^3 and its composition was approximated by 100% Zr. The unit cell geometry is assumed to be square for both oxide and hydride fuel lattices.

Tables 2 and 3 compare the k_∞ values calculated for the oxide and hydride fuel lattices. The agreement between the three codes is satisfactory. The codes also agree very well – within 1%, on the neutron flux amplitude prediction. Larger discrepancies were found in the prediction of certain reaction rates, but reaction rate ratios are in good agreement.

The results presented in Table 3 also show that using the free gas model for the fuel hydrogen scattering kernel overestimates k_∞ by ~1%. Table 3 also shows that cylindricalization of the hydride unit cell is a good approximation.

Table 1 Dimensions and composition of the reference unit cells

	UO_2 (10.4215 g/cm^3)	U-$ZrH_{1.6}$ (8.256 g/cm^3)
Outer Radius (cm)		
Fuel Pin	0.4095	0.59903
Gap	0.4178	0.60411
Clad	0.4748	0.64475
Water	0.7109	0.7109
HM inventory (g/cm)		
5% enrichment: ^{235}U	0.2420	0.209
^{238}U	4.5971	3.979
Total	4.8391	4.188
7.5% enrichment: ^{235}U	0.3629	0.314
^{238}U	4.4762	3.874
Total	4.8391	4.188
10% enrichment: ^{235}U	0.4839	0.4188
^{238}U	4.3552	3.7692
Total	4.8391	4.188

Table 2 k_∞ comparison for reference PWR unit-cell of UO_2 fuel (5w/o enrichment)

	MCNP4B2	WIMSD-5B		SCALE 4.4	
	Square	Cylindrical	Δk_∞	Cylindrical	Δk_∞
k_∞	1.423029±0.00083	1.43130	0.58%	1.42445	-0.1%
Library	Continuous ENDF/B-V At 300 K	69-group WIMS At 300 K		44-group based on ENDF/B-V; 300 K	

Table 3 k_∞ comparison for reference PWR unit-cell of U-$ZrH_{1.6}$ fuel

	MCNP4B2		WIMSD-5B		SCALE 4.4 (SAS2H)	
	Square	Cylindrical	Cylindrical	Δk_∞	Cylindrical	Δk_∞
k_∞	1.42946 ±0.00073	1.43110 ±0.0026	1.43865	0.5%	1.42451	-0.3%
Library	Continuous ENDF/B-V		69-group WIMS		44-group based on ENDF/B-V	
Scattering Treatment	S(α,β); h/Zr.05t at 800 K[a]		H - I.D. 3001[b]		H in ZrH_2 I.D. 1701[c]	

[a] Without S(α,β) and at 300 K fuel temperature k_∞ = 1.44597±0.00072.
[b] No modified scattering data available for H in Zr hydride.
[c] Almost no difference in k_∞ between I.D. 1001 & 1701

4. Results

4.1 Optimal P/D Ratio

Figures 1 and 2 compare the hydride versus oxide fuel k_∞ dependence on the lattice pitch-to-diameter (P/D) ratio for three burnup levels; one for 5% and the other for 10% enrichment. The fuel rod dimensions are those reported in Table 1 for oxide fuel so that the variable is, actually, the pitch. An extended parametric study showed that, for a given P/D, k_∞ is practically independent of the fuel rod diameter. The fuel, clad and water average temperatures were assumed to be, respectively, 978 K, 607 K and 579 K. The vertical dashed red line denotes the P/D ratio (1.326) of the reference oxide fuelled PWR.

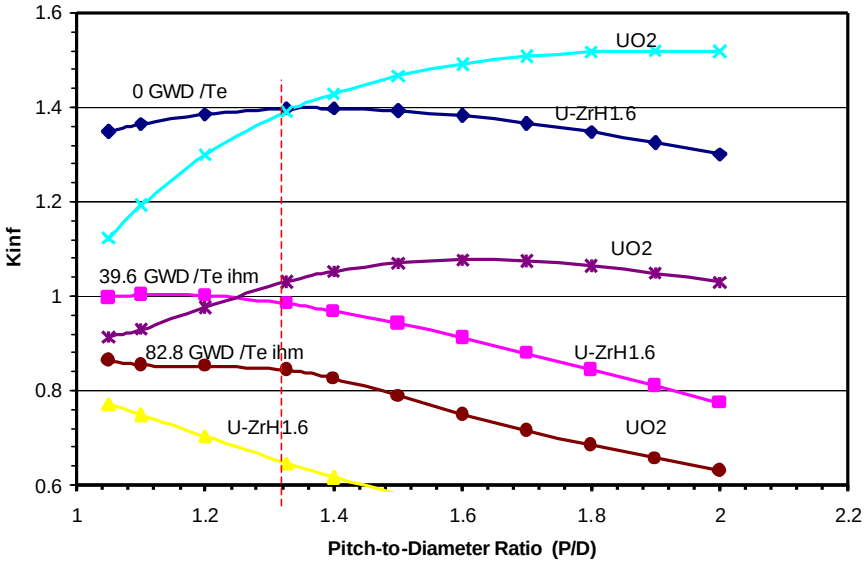

Fig. 1 k_∞ of hydride fuel versus oxide fuel at selected burnup levels as a function of the lattice P/D. Uranium is enriched to 5% ^{235}U.

It is observed that the hydride fuel k_∞ dependence on P/D is significantly flatter than that of oxide fuel, that k_∞ peaks at significantly smaller P/D values and that the peak discharge burnup of hydride fuel is similar to the discharge burnup of the P/D=1.326 oxide fuel. The slope of the k_∞ versus P/D curves near the discharge burnup indicate that (1) the coolant

temperature coefficient (CTC) of reactivity of hydride fuel lattices is of a significantly smaller magnitude than that of oxide fuel lattices and, (2) in order to have negative CTC the hydride fuel lattices should be confined to the P/D < ~1.15 for 5% enrichment and P/D<~1.25 for 10% enrichment.

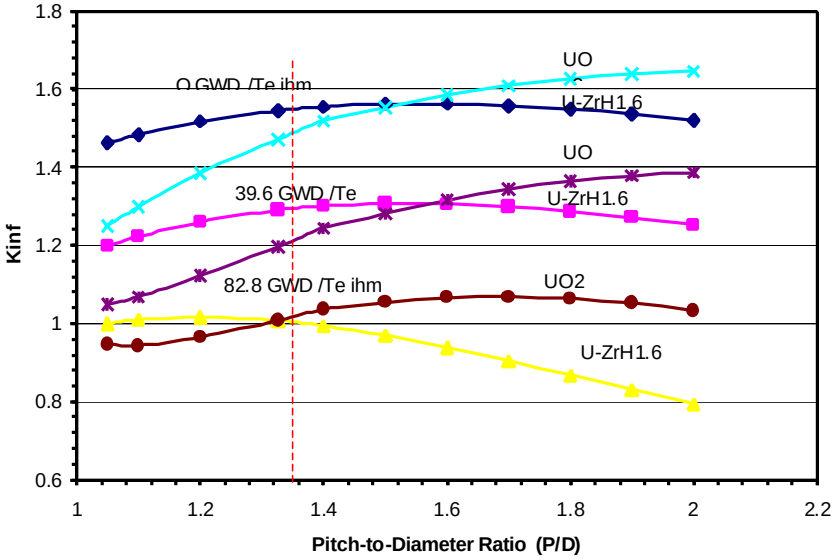

Fig. 2 k_∞ of hydride fuel versus oxide fuel at selected burnup levels as a function of the lattice P/D. Uranium is enriched to 10% ^{235}U.

4.2 Coolant Temperature Coefficient

Figure 3 compares the CTC of hydride versus oxide fuel lattices. It substantiates the above observation concerning the acceptable range of P/D. The temperature dependence of the water density was taken from reference [4]. The magnitude of the CTC is significantly lower than that of oxide fuel lattices. This is illustrated in Table 4. The same trend applies to the void coefficient (Table 4).

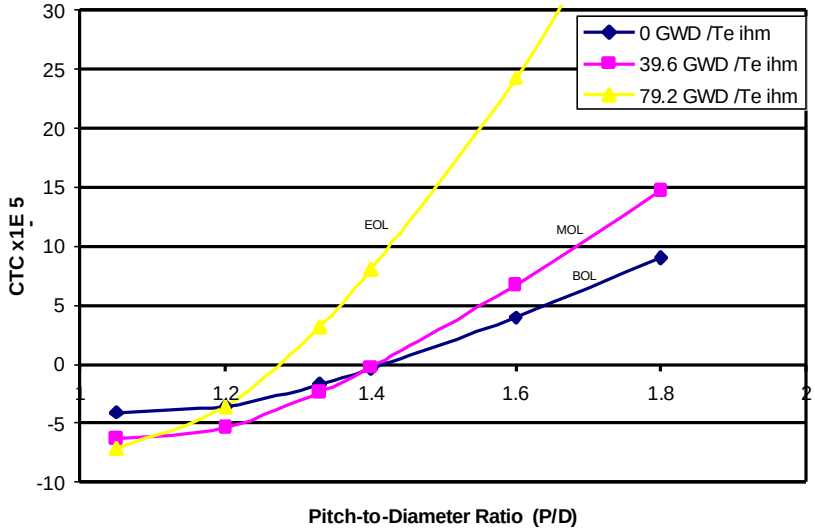

Fig. 3 CTC versus P/D for selected burnups for U-$ZrH_{1.6}$ in square lattice, 10% enrichment.

4.3 Fuel Prompt Temperature Coefficients

Table 4 compares the prompt temperature coefficient of reactivity and other selected characteristics of selected hydride versus oxide fuel lattices for different enrichment levels at beginning (BOL) and end –of-life (EOL). The fuel dimensions are that of the reference oxide fuel cell (Table 1).

Table 4 Selected performance characteristics of representative U-$ZrH_{1.6}$ and UO_2 lattices.

	U-$ZrH_{1.6}$			UO_2		
	5%	7.5%	10%	5%	7.5%	10%
P/D	1.10	1.15	1.20	1.33	1.33	1.33
Loading (g/cm)						
U-235	0.0979	0.1468	0.1957	0.2420	0.3629	0.4839
U-238	1.8593	1.8104	1.7615	4.5971	4.4762	4.3552
Total HM	1.9572	1.9572	1.9572	4.8391	4.8391	4.8391
Zr	2.2815	2.2815	2.2815			
H	0.0412	0.0412	0.0412			
0				0.6511	0.6511	0.6511
H (in water)	0.0298	0.0377	0.0459	0.0684	0.0684	0.0684
Total H	0.071	0.0789	0.0871	0.0684	0.0684	0.0684
H/U-235 (g/g)	0.725	0.537	0.445	0.283	0.188	0.141
H/HM (g/g)	0.0211	0.0211	0.0211	0.0141	0.0141	0.0141
Flux (relative)[a]						
Fast	51.9/52.8		57.2/54.3	61.0/62.8		65.5 /65.8
Resonance	26.3/26.6		27.7/26.5	28.9/29.2		28.8 /29.0
Thermal	21.8/20.6		15.1/ 19.2	9.2/9.0		5.7/5.2
k_∞ (BOL)	1.38472	1.45503	1.51672	1.39118	1.44124	1.47085
BU (GWD/T ihm)	35.7	59.0	80.9	39.8	59.3	77.4
Reactivity coefficients[a] **(pcm or x1E-5)**[b]						
DC+H BOL	-3.3	-2.7	-2.3	-2.0	-1.8	-1.7
EOL	-2.2	-1.6	-1.2	-3.2	-3.1	-3.0
CTC BOL	-3.2	-3.4	-3.5	-10.7	-10.6	-10.2
EOL	-3.8	-3.7	-3.6	-17.1	-19.2	-19.7
VC BOL	-18.2	-27.3	-35.8	-115.0	-110.5	-102.2
EOL	-52.2	-63.4	-75.2	-201.2	-202.6	-202.7

[a] Energy group boundaries are at 0.625 eV and 15.03 KeV. X/Y stands for BOL/EOL.
[b] DC+H = prompt fuel feedback (Doppler coefficient + H heating); VC = Void coefficient.

It is observed that at BOL the U-$ZrH_{1.6}$ fuel prompt reactivity coefficient (DC+H) is significantly more negative than that of oxide fuel lattices. The magnitude of the hydrogen-induced spectrum hardening (H) is of the order of 20% of the total (DC+H). However, at EOL the trend is reversed – hydride fuel has a smaller magnitude, although negative, prompt reactivity coefficient than oxide fuel. Interestingly, whereas the magnitude of DC+H increases with burnup for oxide fuel, it decreases for hydride fuel. The spectrum hardening due to fuel temperature increase, practically absence in case of oxide fuel, enhances the neutron absorption probability in the ~0.3 eV resonance of ^{239}Pu.

Notice (Table 4) that the spectrum of the hydride and oxide fuel lattices is quite different – having larger total hydrogen-to-^{235}U atom ratio (Table 4), the hydride fuel has a softer spectrum.

The inclusion of Erbium burnable poison in the fuel can significantly increase the prompt hydrogen negative temperature coefficient of reactivity. This enhancement effect, due to the large double resonance of Erbium at ~0.5 eV, is illustrated in Table 5.

Table 5 Effect of erbium on hydride fuel prompt temperature coefficient of reactivity. 10% enrichment. Reference oxide unit cell geometry (Table 1)

Fuel Reactivity Coefficient	$U\text{-}ZrH_{1.6}$	$U\text{-}ZrH_{1.6}$ + 0.9 $^{w}/_{o}$ erbium
Total	$-2.33\times10^{-5}\pm 0.05\times10^{-5}$	$-4.28\times10^{-5}\pm 0.09\times10^{-5}$
Hydrogen in Zirconium	-0.49×10^{-5} (21%)	-2.18×10^{-5} (51%)

4.4 Fuel Delayed Temperature Coefficient

Figure 4 shows the effect of the hydrogen-to-zirconium atom ratio on k_∞ for hydride fuel lattices of selected P/D ratios. The uranium is enriched to 10%. It is observed that the slope of the k_∞ versus x plots is positive for P/D < ~1.25 and negative for larger P/D values. This implies that as long as P/D < 1.25, dissociation of hydrogen due to fuel temperature increase followed by diffusion of the free hydrogen out of the fuel (say, into the fission gas plenum) will result in a loss of reactivity. This is a mechanism for introducing a negative reactivity feedback that is unique to hydride fuel. As the hydrogen diffusion process is slow relative to the neutron generation time, this reactivity feedback mechanism is a delayed one.

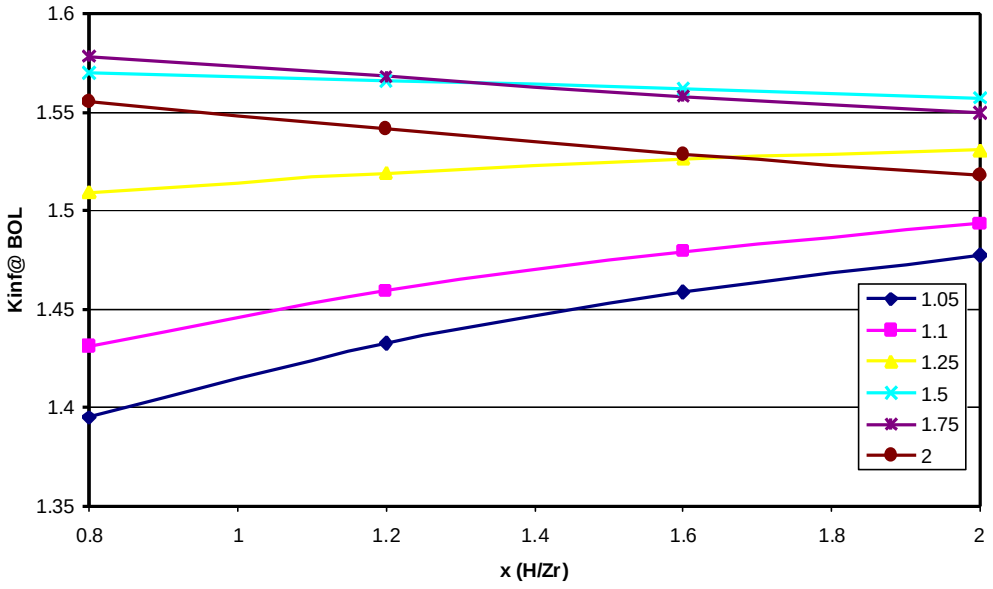

Fig. 4 Effect of hydrogen-to-zirconium atom ratio on k_∞ of hydride fuel lattices of different P/D ratios. 10% enrichment.

4.5 Criticality Safety Considerations

Infinite lattice calculations were also carried out in absence of water for different enrichment levels. It was found that the k_∞ of the $U\text{-}ZrH_{1.6}$ lattices exceeds 1.0 at an enrichment level of 1.63 $^{w}/_{o}$. The corresponding enrichment level for UO_2 fuel is 7.88 $^{w}/_{o}$.

Consequently, the handling of hydride fuel will require special care; the design of the different type of fuel handling and containing facilities will have to be carefully reviewed and, probably, revised. Nevertheless it is expected that by proper incorporation of neutron absorbers within the fuel handling and containing equipment it will be possible to assure criticality safety in the hydride fuel cycle.

5. Conclusions

The infinite lattice neutronic parametric study indicates that it should be possible to design PWR cores using U-$ZrH_{1.6}$ fuel to have comparable discharge burnup as attainable using UO_2 fuel of the same enrichment. The optimal hydride fuel P/D ratio is significantly smaller than that of oxide fuel. This enables to increase the fraction of the core volume occupied by the fuel and thus to make up for much of the HM density disadvantage of U-$ZrH_{1.6}$.

U-$ZrH_{1.6}$ fuelled cores can be designed to have negative coolant and fuel temperature coefficients of reactivity. Whereas at BOL the prompt fuel temperature coefficient of hydride fuel is significantly more negative than that of oxide fuel, the trend is reversed at EOL.

Hydride fuel offers a couple of unique fuel temperature dependent reactivity feedback mechanisms – a prompt feedback due to fuel hydrogen upscattering of low energy neutrons, and a delayed feedback due to hydrogen dissociation and diffusion out from the fuel.

Careful attention to criticality safety will have to be given when handling U-$ZrH_{1.6}$ fuel.

Acknowledgment

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References

1) WIMSD-5B (98/11), "Deterministic Code System for Reactor-Lattice Calculations", RSICC CCC-656, user manual (1998).
2) J.F. Briesmeister, editor, "MCNP4B2- A General Monte Carlo N-Particle Transport Code, Version 4B2", RSICC CCC-660, user manual (1999).
3) "SAS2H: A Coupled One-dimensional Depletion and Shielding Analysis Module" NUREG/CR-0200 Revision 6 (1998).
4) R. D. Mosteller and L. D. Eisenhart, Nucl. Sci. and Eng., 107, pp.265-271, 1991.
5) Zeev Shayer "Neutronic Parametric Analysis: U-$ZrH_{1.6}$ Unit Cell in PWR NERI Project – Rev.4" NERI02-189-TM 2 (2003)
6) Z. Shayer and E. Greenspan, "Preliminary Assessment of Possibilities for Improving the Performance of SCWR Using Hydride Fuel," Submitted for Transactions American Nuclear Society, Pittsburgh, PA, June (2004)