

# Demonstration of the Compact Depletion Models for Burnup Calculations

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## Abstract

We describe a compact depletion model for reactor burnup calculations employing dynamically generated pseudo nuclides in transmutation chains. The model uses microscopic cross sections and number densities of pseudo nuclides calculated by fitting the evolution of pseudo nuclides to reaction rates of explicitly treated nuclides. Functionalisation of the effective yields and effective capture fractions with respect to core state variables is possible, based on results of detailed depletion calculations for scenarios typical for the fuel in a particular reactor. A compact depletion model is employed within the BOLD VENTURE code (Vondy, 1981) used for fuel management calculations of the Hoger Onderwijs Reactor (HOR) at the Interfaculty Reactor Institute (IRI) of the Delft University of Technology.

## 1 Introduction

Basically, there are two depletion models employed for reactor core analyses: macroscopic and microscopic depletion.

In the first model, macroscopic cross sections are parameterised for the expected range of “core state variables” (moderator temperature, density, fuel temperature, Xe density). In addition, the model relies on so called “fuel history state” variables. During reactor operation and fuel depletion, local cross sections do not depend only on current values of core state variables, but also on their previous values. This dependency is a consequence of differences in the spectral history of the fuel. Thus for the same exposure level, we can have different isotopic densities, and different macroscopic cross sections. Fuel history state variables for the macroscopic depletion model are usually constructed by time (or burnup) averaging of the core state variables.

In the microscopic depletion model, the fuel history state is represented through the actual number densities of the nuclides. A typical model for global core calculations includes about 20 to 30 major nuclides and fission products, plus a representation for the effect of the rest of the non-treated nuclides. In the microscopic depletion model, the lattice physics code calculates the broad group microscopic cross sections as a function of core state variables, and the evolution of lumped nuclides as a function of exposure and the atomic densities of the nuclides contained in the lumped nuclide. Figure 1 depicts the application of a microscopic depletion model in global core calculations.

In the past, a macroscopic depletion model was favoured since it avoids solving the depletion equations and it requires less memory. However, with modern fuel designs using higher enrichments, mixed oxide fuels, special operational procedures (spectral shift), functionalisation of macroscopic cross sections is becoming quite complex, because cross sections become more sensitive to the fuel history state variables (Ida, 1996), (Kelly, 1995). The microscopic depletion model provides accurate knowledge of the spatial nuclide density field, which is a big advantage. Therefore, many of the existing macroscopic depletion models are modified or supported by explicit modelling of the evolution of the important nuclides (Lindahl, 1996), (Moon, 1995).

This work describes a microscopic depletion model in which the number of explicitly treated nuclides and lumped pseudo nuclides is less than 20. These pseudo nuclides are different from the traditionally used pseudo nuclides based on non, slow, and rapid saturation (Hoogenboom, 1996). Furthermore, this model contains a few pseudo nuclides that preserve the capture and fission rates of all nuclides not explicitly treated. The densities of the pseudo nuclides can be calculated. This is achieved by including the production of the pseudo nuclides in the transmutation chains of the nuclides explicitly treated with rather small computational effort, even if detailed spatial (node-wise) depletion is performed. Functionalisation of the transmutation parameters for pseudo nuclides is therefore crucial for the application of the concept in global core calculations. We will refer to this concept further on as the Compact Depletion Model (CDM).

## 2 Methodology

CDM is developed by functionalisation of the transmutation parameters (fission yields, capture rates) to preserve accurately pre-calculated nuclide densities in typical fuel depletion scenarios. For accurate cell depletion calculations, we have used the recently developed SAS6 sequence (de Leege, 1995).

In SAS6 the reaction rates of non-treated nuclides are accounted for by six pseudo nuclides. Each of these pseudo nuclides has only a capture cross section or a fission cross section in the thermal, epithermal, or fast energy range as in the three energy group structure employed by the ORIGEN-S code (SCALE-4.2). Given the list and cross sections of the non-treated nuclides, SAS6 calculates the number densities of the pseudo nuclides for each depletion step.

Each pseudo nuclide (either capturer or fissioner) has an identical cross section obtained by weighting a  $1/v$  cross section normalised to 1 barn at 2200 m/s for the thermal and epithermal energy group, and a constant cross section of 1 barn for the fast energy group. Using this artificially designed cross sections ( $\sigma_{1/v}^g$ ), the number densities of pseudo nuclides are determined according to the following relation:

$$N_{PS} = \frac{\sum_i \sigma_i^G \cdot N_i \cdot \Phi_G}{\sum_g \sigma_{1/v}^g \cdot \phi_g} \quad (1)$$

$$\sigma_{PS}^G = \frac{\sum_g \sigma_{1/v}^g \cdot \phi_g}{\sum_g \phi_g}$$

where  $\Phi_G$  represents the ORIGEN-S broad group flux value and  $\sigma_i^G$  the broad group cross section of the particular nuclide  $N_i$  which is to be included in the pseudo nuclide.  $\sigma_{1/v}^g$  is the fine group  $1/v$

cross section and  $\phi_g$  (Maxwell,  $1/E$ , Fission) the fine group flux over the same broad group energy interval, normalised to the same total value as  $\Phi_G$ .

The advantage of this representation is that  $\sigma_{PS}$  is only group dependent. All other effects are reflected in artificially designed number densities of the pseudo nuclides.

## 2.1 Development of compact depletion models

The applicability of the CDM concept was tested using SAS6 cell depletion calculations as a reference model.

The output of SAS6 contains all necessary quantities to define and test CDM: stepwise values of nuclide densities, one-group microscopic cross sections, and absolute fluxes. These data are automatically extracted and used as input to the new CDM module, which simulates the reference cell depletion using a compact chain representation specified by the user. The solution of the depletion equations in the CDM module is based on finite difference and higher order generation rate formulation (Vondy, 1981). This module also determines the effective transmutation parameters (reaction rates – yields, capture fractions) of the pseudo nuclides in order to match the reference nuclide density evolution over the given period. Using the reaction rates of the major nuclides obtained by the CDM module, the transmutation parameters are fitted to reproduce the evolution of nuclides calculated by SAS6. The transmutation parameters are fitted by a modified Levenberg-Marquardt method (Press, 1989).

In this way, the effective transmutation parameters for the fuel could be determined for a number of different depletion scenarios with respect to important fuel state or history variables (e.g. control rod insertion, void fraction, or spectral ratio).

In general, the complexity of CDM depends on the fuel considered. For some fuels a greater number of explicitly treated nuclides will be needed in order to reproduce number densities within certain error margins, while keeping functionalisation of transmutation parameters as simple as possible. Compared with a macroscopic depletion model, in CDM the influence of fuel history effects is only accounted for in the densities of the pseudo nuclides. On the other hand, the evolution of pseudo nuclides is related to the reaction rates of the explicitly treated nuclides, which should further diminish parameterisation with respect to history variables.

The CDM concept was tested using 13 explicitly treated nuclides: four uranium nuclides, ( $^{234}\text{U}$ ,  $^{235}\text{U}$ ,  $^{236}\text{U}$ ,  $^{238}\text{U}$ ), three plutonium nuclides ( $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ ) nuclides, and six major fission products: ( $^{135}\text{I}$ ,  $^{135}\text{Xe}$ ,  $^{149}\text{Pm}$ ,  $^{149}\text{Sm}$ ,  $^{151}\text{Pm}$ ,  $^{151}\text{Sm}$ ). The rest of the capture and fission reaction rates are represented by six pseudo nuclides. Generic relations among nuclides are depicted in Figure 2. Two different reactor types with different depletion scenarios were used for testing the model:

1. Research reactor fuel depletion scenarios (high enriched (93%) uranium (HEU) and low enriched (20%) uranium (LEU) of the HOR reactor):
  - Normal fuel cell (thermal spectrum)
  - Control rods fuel cell (hard spectrum)
  - Fuel cell in the neighbourhood of a control rod (soft spectrum)
  - Simulation of control rod insertion and withdrawal
2. BWR fuel (Kelly, 1995)
  - Depletion with different void fraction histories

Purpose of the testing was to study the complexity and accuracy of the CDM functionalisation for different fuel types in different regions of the core. For both fuel types the core state variables with large impact on isotopic evolution were chosen (control rod insertion for research reactor fuel and void fraction for BWR fuel). In the following section the evolution of pseudo nuclides and their (possible) functionalisation is described.

### 3 Results

Figure 3 shows the relative contributions of the capture and fission reaction rates of pseudo nuclides during the depletion under different circumstances. Except for the fast capturer pseudo nuclide whose contribution can practically be neglected, depletion of all other pseudo nuclides should be accurately modelled. The effect of the pseudo fissioners is smaller the more fissile isotopes are explicitly treated and in the case of higher enriched fuel.

Almost linear build-up of the two most important pseudo nuclides, thermal and epithermal capturer, reveals that fission products are their major contribution. This means that effective fission yields could be sufficient to accurately describe their build-up. The pseudo fissioners number densities change exponentially, and effective capture fractions from nuclides like  $^{241}\text{Pu}$  and  $^{236}\text{U}$  can be used to describe their behaviour.

Calculations have shown that using capture reactions by  $^{241}\text{Pu}$  and  $^{236}\text{U}$  as two other sources of pseudo captureurs improves the accuracy of the model on the expense of a more complex functionalisation. Figure 4 shows the effective yields for the two pseudo captureurs obtained by the CDM module as a function of the spectral ratio (fast flux/thermal flux) in high enriched and low enriched fuel of the HOR. Unlike real nuclides, the effective yields of pseudo nuclides change significantly with the spectrum, which is a consequence of the assumptions expressed in Eq. (1). The figure indicates almost a linear relationship, which suggest that effective yields for two pseudo captureurs for the HOR fuel can be functionalised as:

$$y_{eff}^L = a \cdot (\phi_1 / \phi_2) + b \quad (2)$$

where

$L$  – different enrichment/type of fuel

$\phi_1/\phi_2$  – spectral ratio (fast to thermal flux)

In order to study the impact of the depletion history on the effective yields of pseudo nuclides, we have defined two different depletion scenarios shown in Figure 5. The pseudo capturer's evolution against a detailed SAS6 calculation using effective yields according to Eq. (2) is shown in Figure 6. A similar kind of testing has been done for a typical BWR fuel cell for several depletion scenarios with a significant variation of the void fraction during depletion. For illustration, two scenarios are depicted in Figure 7a, while Figures 7b and 7c show the spectral ratio and its historical average for the two scenarios. The effective yields for the two scenarios were fitted within depletion intervals having the same void fraction. The effective yields as a function of the average value of the spectral ratio within intervals are shown in Figure 8. Again, the effective yield shows a strong dependence to the void fraction or spectral ratio. It is obvious that the dependence on depletion history is a second order effect, especially in the case of the epithermal pseudo capturer. However, in order to describe the evolution of the pseudo nuclides more accurately, functionalisation of the effective yields of pseudo captureurs should be done both with respect to important core state variables and their historical values.

In practice, effective yields (and capture fractions) can be tabulated and reconstructed by interpolation for any particular core state, as is done with the correction factors of macroscopic cross sections within the macroscopic depletion models.

Figure 9 shows the reconstructed evolution of the pseudo nuclides versus the original values of the SAS6 calculation, using the effective yields depending only on the current value of the spectral ratio. As in Figure 6 one can observe a step change in the nuclide number density at the point of the abrupt change of the spectral parameter. This is a consequence of the definition of  $\sigma_{PS}$  ( $=\sigma_{1/v}$ ). As the macroscopic cross section of all the nuclides contained in the epithermal capturer is not behaving as a  $1/v$  cross section in the resonance part of the spectrum, the difference is reflected in the pseudo nuclide's number density. This means that this step change in pseudo nuclide number density must also be functionalised with respect to the spectral ratio (or core state variables).

Capture reactions of  $^{241}\text{Pu}$  and  $^{236}\text{U}$  were used as a source for the pseudo fissioners, and the effective capture fractions were fitted using the CDM fitting procedure. Similarly to the effective yield model, the effective capture fractions have to be functionalised with respect to the void fraction or spectral ratio.

### 3.1 *Application of CDM in the global depletion calculation for the HOR reactor*

The fuel management calculations for the HOR reactor are performed using the finite difference diffusion code BOLD VENTURE. Both two- and three-dimensional models are used based on five energy groups (microscopic cross section library). Using the exposure module of BOLD VENTURE it is possible to implement the compact microscopic depletion model in the HOR calculations. The microscopic cross sections of the fuel nuclides in the library are dependent on fuel type and burnup. This representation takes into account spectrum changes that are related to burnup of the fuel and are reflected on the cross sections. It also allows functionalisation of the transmutation parameters with respect to the burnup and fuel type, which is significant for the implementation of the microscopic depletion model. The effective yields and capture fractions for the pseudo nuclides are shown in Table 1. The accuracy of the employed CDM model for the HOR depletion calculations is well within 1% for the number densities of the major nuclides ( $^{235}\text{U}$ ,  $^{238}\text{U}$ ), and typically within 5% for the pseudo nuclides. CPU time consumption for the zone-wise exposure calculation is typically within 10% of the time needed for the flux calculation.

## 4 **Conclusions**

Fuel management of modern reactor types involves depletion of fuel with diverse neutronic characteristics in spectrally different and/or changing environments. Calculation of depletion induced changes using a macroscopic depletion approach may be inadequate due to strong fuel history effects. The compact depletion model described here, provides explicit calculation for the major nuclides and lumped pseudo nuclides using effective transmutation parameters fitted to the reaction rates of major nuclides. The model is a useful extension to transmutation chains as used in global core burnup calculations. The model is independent of the number of major nuclides used. Detailed lattice depletion calculations using the SAS6 code system are used to determine the pseudo nuclides effective transmutation parameters.

The main advantage of CDM is a more accurate treatment of the burnup history effects in global core calculations. Since the major nuclides are explicitly treated, the burnup history parameterisation is limited to the pseudo nuclides and therefore, errors in the depletion calculations

are mainly due to uncertainties in the pseudo nuclide density calculations. The compact depletion model is used for the burnup calculations of the HOR research reactor.

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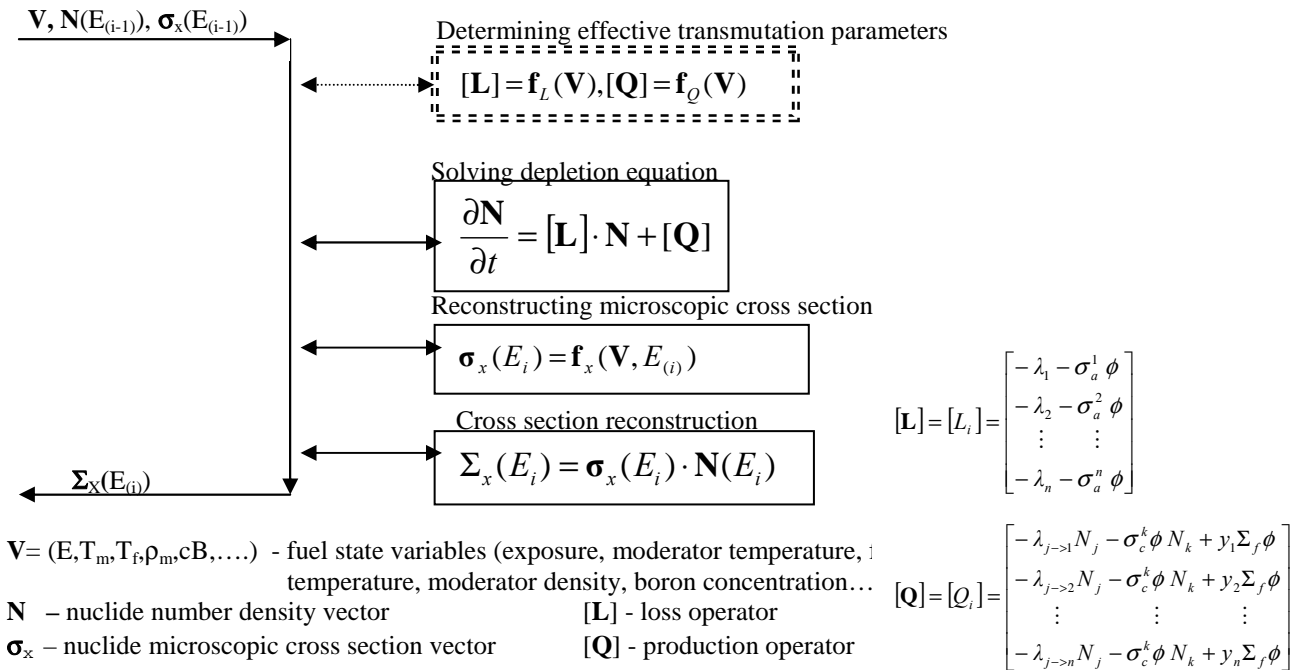


Fig.1 Microscopic depletion and cross section reconstruction model. Dashed box indicates additional part for the compact depletion model (CDM), i.e. determination of effective parameters for the particular depletion step. Although this is an additional step, CDM is much faster in depletion calculation due to smaller dimensions ( $[\mathbf{N}], [\mathbf{L}], [\mathbf{Q}]$ ).

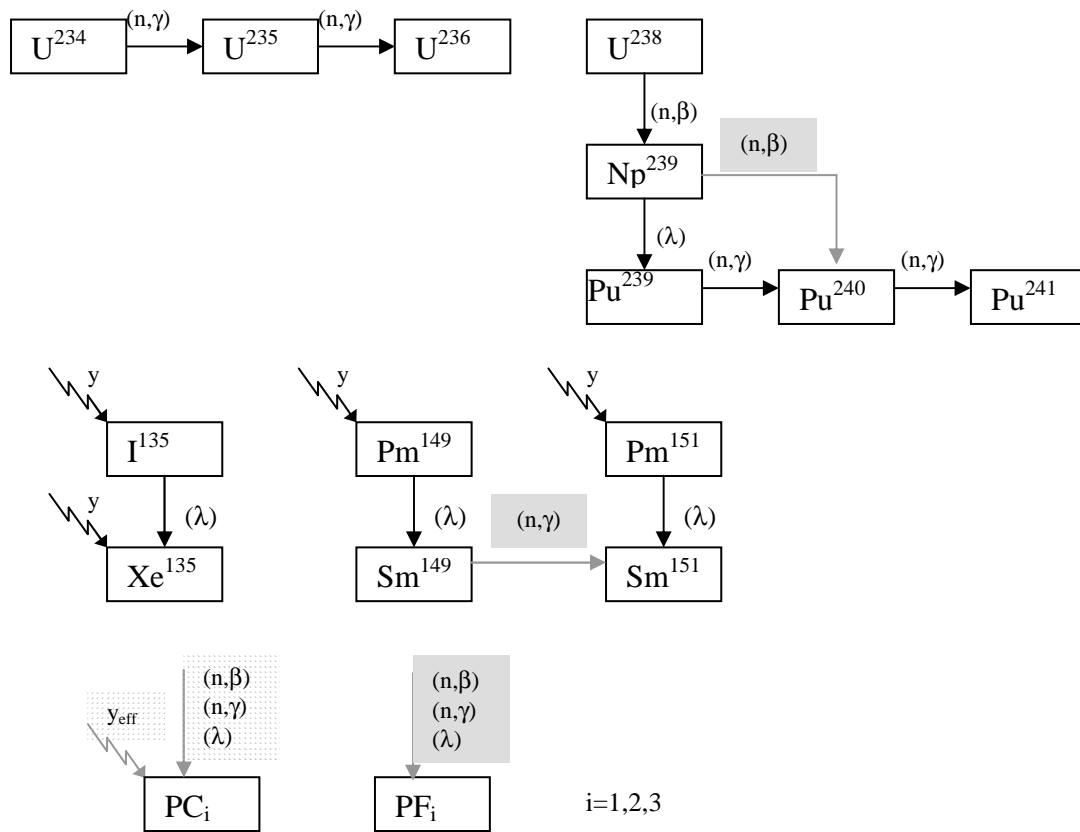


Fig. 2 Generic compact depletion model. Reactions in shadow indicate artificial effective reactions, which can be functionalised with respect to core state variables in order to produce correct number densities of the related nuclide.

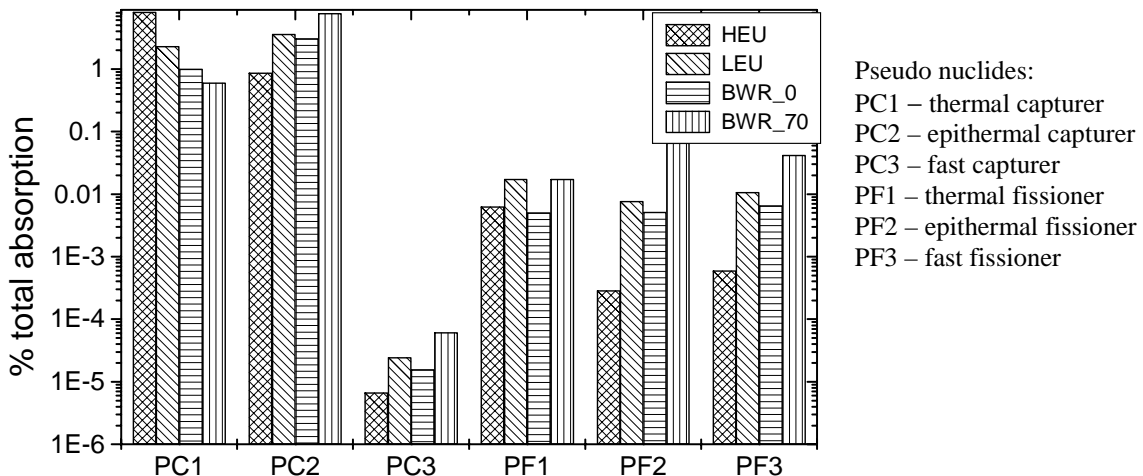


Fig. 3 Contribution of the pseudo nuclides in reaction rates for different types of fuel: HEU and LEU fuel for the HOR at the end of life (70% burned  $^{235}U$ ), BWR fuel (70% void fraction and 0% void fraction) after three years at full power.

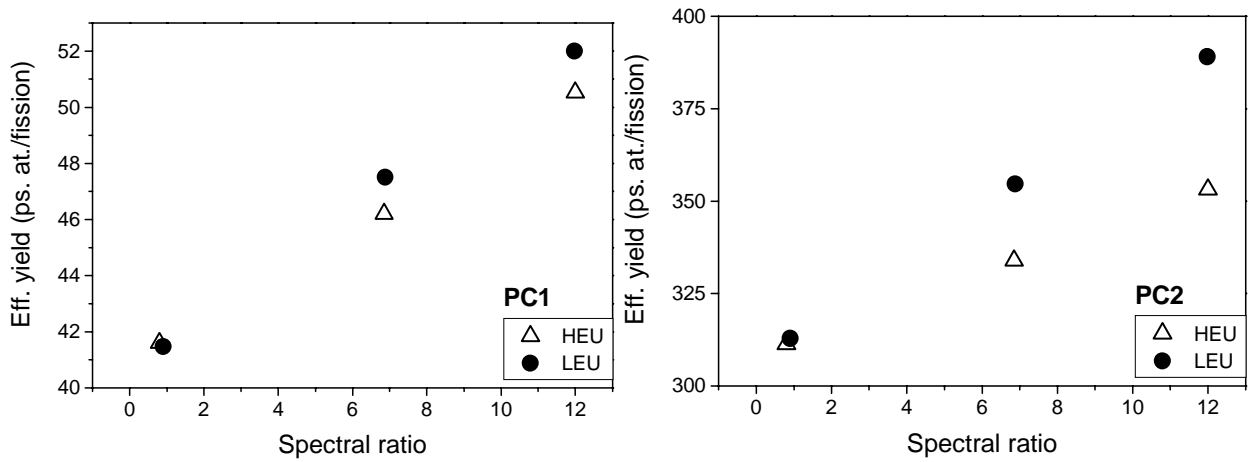


Fig. 4 Effective yields for thermal and epithermal pseudo capturer (PC1 and PC2) vs. spectral ratio for HOR fuel determined for the whole burnup range.

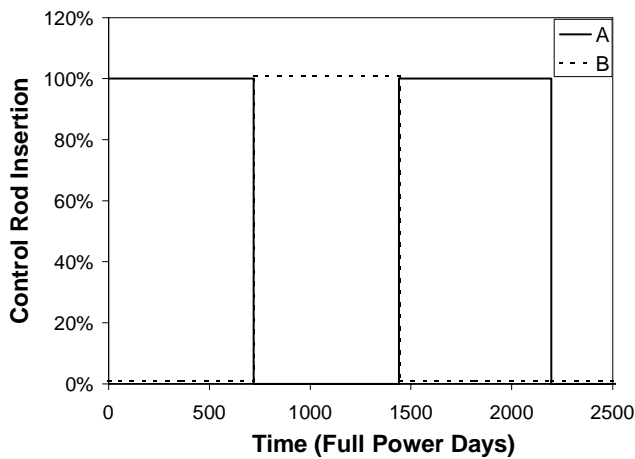


Fig.5 Control rod insertion for two depletion scenarios, HOR fuel.

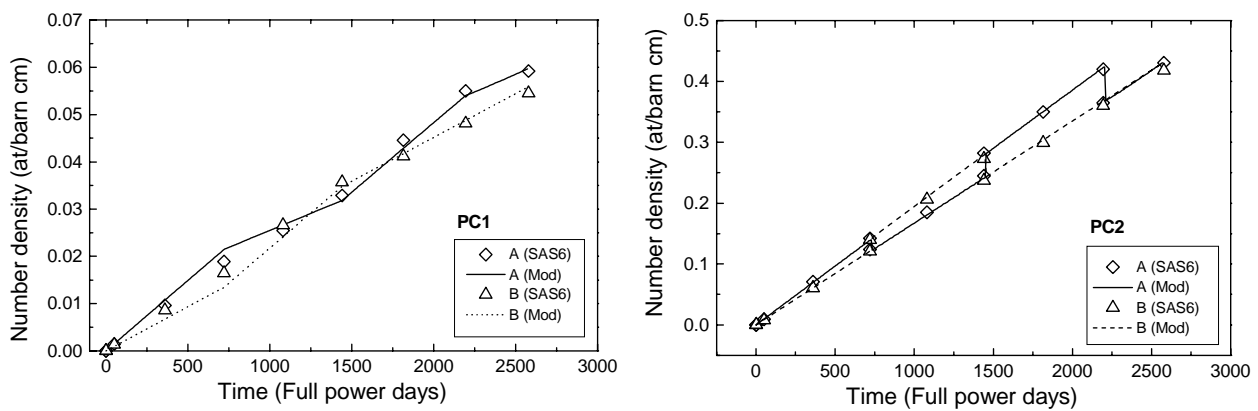


Fig. 6 Evolution of thermal (PC1) and epithermal pseudo capturer (PC2) for the HOR LEU fuel; detailed model (SAS6), vs. effective yield reconstruction.

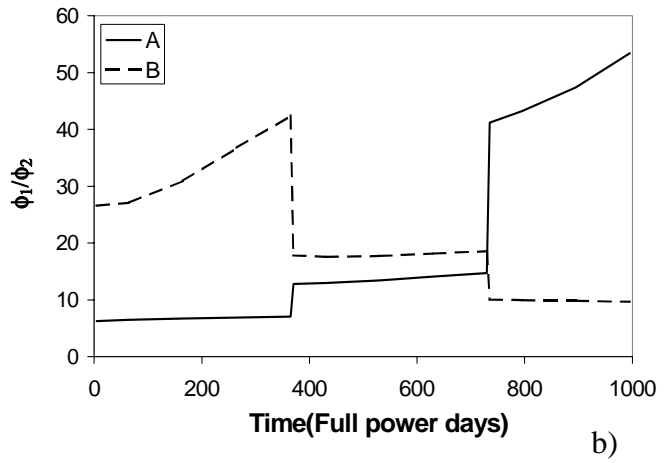
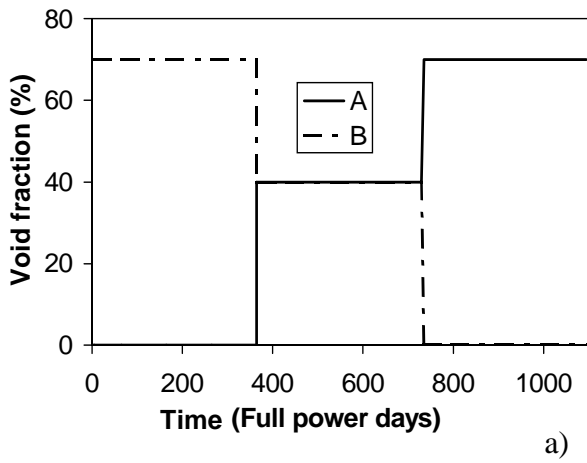


Fig. 7 BWR depletion scenarios.  
 a) void fraction vs. time  
 b) spectral ratio vs. time  
 c) historical value of spectral ratio vs. time

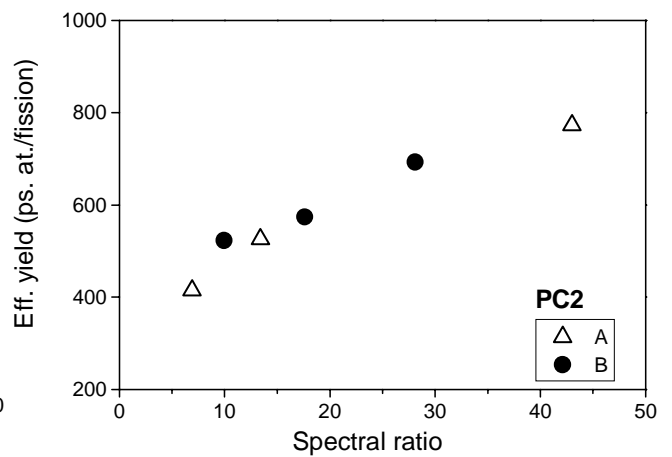
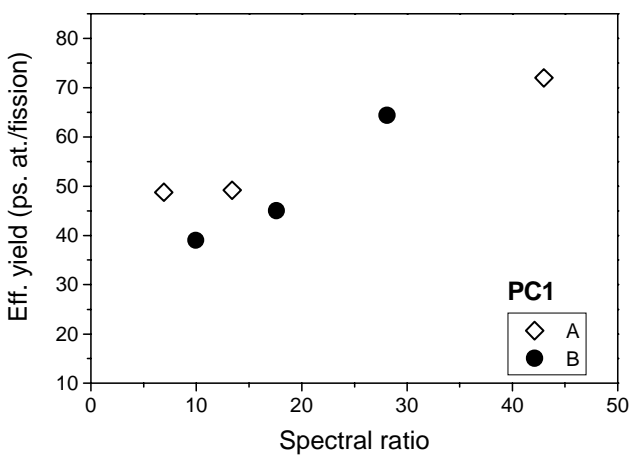
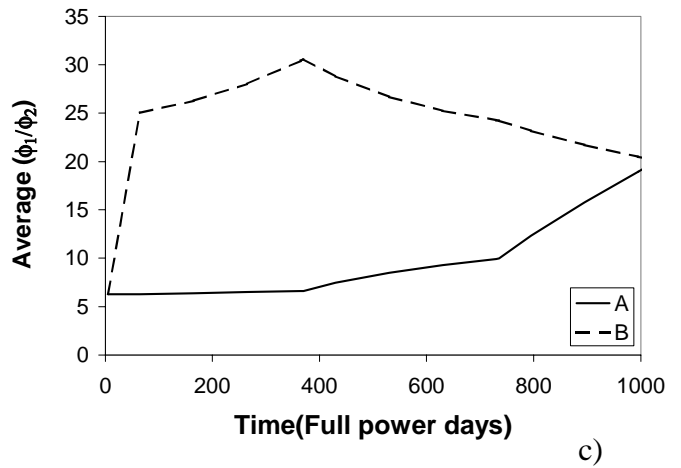


Fig. 8 Effective yields for the thermal pseudo capturer (PC1) and epithermal pseudo capturer (PC2) as a function of the spectral ratio for BWR fuel in two depletion scenarios.

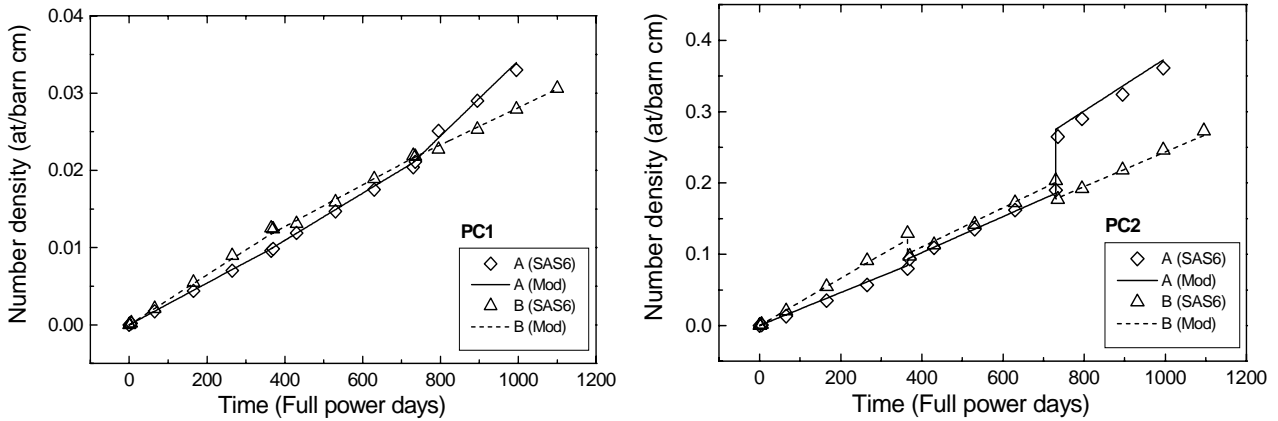


Fig. 9 Evolution of the-thermal and epithermal pseudo capture rates (PC1 and PC2) for two BWR fuel depletion scenarios, detailed model (SAS6) vs. effective yield reconstruction. Good correspondence between CDM and accurate SAS6 calculations.

Table 1 Effective yields and capture fractions for the HOR research reactor fuel as determined by CDM module fitting. Effective yields are determined and tabulated for burnup intervals (max. and min. values are indicated in the Table), while effective capture fractions for pseudo fissioners are constant and determined for the whole burnup range. Accuracy is indicated as maximum error in % nuclide density (ND) for the whole burnup range.

Pseudo nuclide	Transmutation parameter	Values	Accuracy ( $\Delta$ ND %)	Functionalisation
<b>HEU</b>				
PC1	$y_{\text{eff}}$	48 – 32	$<\pm 4\%$	burnup dependent
PC2	$y_{\text{ef}}$	315 – 270	$<\pm 5\%$	burnup dependent
PC3	$y_{\text{ef}}$	3.30E-04 - 1.35E-04	$<\pm 10\%$	burnup dependent
PF1	$c_{\text{eff}}^{\text{Pu}^{241}}, c_{\text{eff}}^{\text{U}^{236}}$	940 ; 1.72	$<\pm 5\%$	constant
PF2	$c_{\text{eff}}^{\text{Pu}^{241}}, c_{\text{eff}}^{\text{U}^{236}}$	2300 ; 12.1	$<\pm 5\%$	constant
PF3	$c_{\text{eff}}^{\text{Pu}^{241}}, c_{\text{eff}}^{\text{U}^{236}}$	22.8 ; 1.63	$<\pm 5\%$	constant
<b>LEU</b>				
PC1	$y_{\text{eff}}$	49 – 33	$<\pm 4\%$	burnup dependent
PC2	$y_{\text{ef}}$	320 – 280	$<\pm 6\%$	burnup dependent
PC3	$y_{\text{ef}}$	1.45E-04 - 5.90E-05	$<\pm 10\%$	burnup dependent
PF1	$c_{\text{eff}}^{\text{Pu}^{241}}, c_{\text{eff}}^{\text{U}^{236}}$	49.5 ; 1.61	$<\pm 5\%$	constant
PF2	$c_{\text{eff}}^{\text{Pu}^{241}}, c_{\text{eff}}^{\text{U}^{236}}$	85.7 ; 13.2	$<\pm 5\%$	constant
PF3	$c_{\text{eff}}^{\text{Pu}^{241}}, c_{\text{eff}}^{\text{U}^{236}}$	1.91 ; 1.77	$<\pm 5\%$	constant

$y_{\text{eff}}$  - effective yield

$c_{\text{eff}}$  - effective capture fraction.