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Application of Heterogeneous Depletion Scheme in Pin-by-Pin Core Simulator SPHINCS

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1. Introduction

SPHINCS [1] is a pin-wise neutronics code based on the finite difference solution of the SP_3 equations. With the nTRACER [2] generated pin cell cross sections, SPHINCS performs the core calculation including depletion calculation with pin-wise isotopic number densities and microscopic cross sections.

SPHINCS utilizes the SPH [3] method to minimize the pin-homogenization error. This method corrects the flux or reaction rate error originating from homogenization at each pin of an assembly. With those adjusted reaction rates, most of the number densities of the nuclides are calculated accurately. However, this does not hold for gadolinium (Gd) isotopes which are the major burnable poison sources.

Therefore, many neutronics codes utilize the effective Gd depletion model [4], which lumps Gd isotopes into a single pseudo-isotope [5], and achieve sufficient accuracy. However, as the computational resources are getting cheaper, SPHINCS aims to calculate all the Gd isotopes' number densities explicitly.

The issue of heterogeneity within a pin cell which is neglected with pin homogenized models is important at low and middle burnup states, especially when Gd quadratic depletion model [6] is used. To handle the errors from the heterogeneity in depletion problems, heterogeneous depletion calculation functions are added that use the same sptial dicretization as nTRACER.

In the following, the reason and the effect of sub-pin heterogeneity in Gd pins are discussed, and then the enhancements by applying a heterogeneous depletion scheme will be presented.

2. Heterogeneity of Depletion Problem

Although the heterogeneity in depletion problems has not been discussed extensively, clearly there are certain discrepancies between homogeneous and heterogeneous depletion calculations. In most cases, they show very similar results as far as total reaction rates are conserved. However, merely conserving the reaction rate does not always guarantee good accuracy, especially in highly self-shielded regions such as the internal regions of Gd bearing pins.

To obtain the pin-averaged number densities on the next time step, the heterogeneous number densities should be first calculated and then homogenized. This can be formulated as follows:

$$\bar{\mathbf{N}}^{k+1} = \sum_m \left(\exp\left(-\mathbf{A}_m^k \Delta t\right) \mathbf{N}_m^k \frac{V_m}{V_{total}} \right) \quad (1)$$

where k is the index of depletion step; m is the index of the heterogeneous region within a pin referred to as flat cross section region (FXR); $\mathbf{N}$ is the heterogeneous number density vector; $\mathbf{A}$ is the heterogeneous burnup matrix and V is the volume of the region.

However, SPHINCS has only homogeneous quantities like pin-averaged number densities and pin-wise reaction rates. Therefore, SPHINCS used to set up the depletion systems with the following equation (2):

$$\bar{\mathbf{N}}^{k+1} = \exp\left(-\bar{\mathbf{A}}^k \Delta t\right) \bar{\mathbf{N}}^k \quad (2)$$

where $\bar{\mathbf{N}}$ is the homogeneous number density vector and $\bar{\mathbf{A}}$ is the homogeneous burnup matrix.

The difference between Eqs. (1) and (2) comes from that of burnup matrices and number density vectors. The heterogeneity in atomic reaction rates causes the discrepancies, resulting in different burnup matrices.

The heterogeneity problem diminishes as the fuel deplete since the reaction rates become uniform over all regions. Thus the heterogeneity problem can be ignored for high burnup states whereas it is important for low burnup states.

To demonstrate the heterogeneity effect, two cases are tested on a Gd bearing fuel pin by varying only the regional discretization level in the nTRACER lattice calculation. The number of FXRs is ten in the heterogeneous case, and the other has only one region. The results show very different error levels. **Figure 1** and **Figure 2** illustrate the multiplication factors with burnup using ten and one FXR in the fuel region, respectively, and the differences in eigenvalue from the corresponding pin-homogenized depletion. As expected, the impact of heterogeneity makes large difference on the low burnup states.

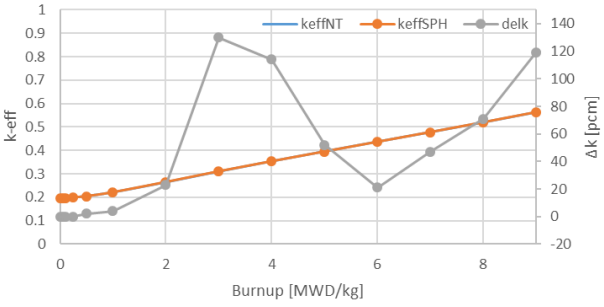

Figure 1. k_{eff} comparison with ten FXRs in the fuel pin.

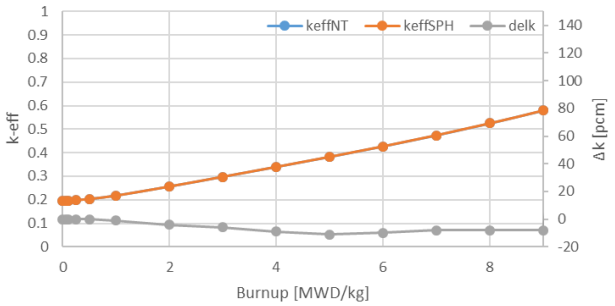

Figure 2. k_{eff} comparison with one FXR in the fuel pin.

To see how large the heterogeneity in a pin cell is and why they affect significantly, we have to examine the fraction of atomic reaction rates and quantities of FXRs. The representative Gd-155 is chosen for comparison.

In **Figure 3** and **Figure 4**, region-wise fractions of atomic reaction rates and the quantities of Gd-155 are presented. The regions are divided equi-volumetrically with rings ranging from R1 to R10. R1 is the outermost one and R10 is the innermost one. Seeing both figures, we can notice that each ring has very different values and derivatives changing with time.

As the spatial variation of the fractions is large during the early depletion stage, the rings should be treated separately. Without any heterogeneous treatment, inner regions will see higher reaction rates while outer regions observe lower reactions rates. This results in faster depletion of Gd isotopes during early burnup steps and slower depletion in middle burnup steps due to the combined effect of spatial and time discretization errors.

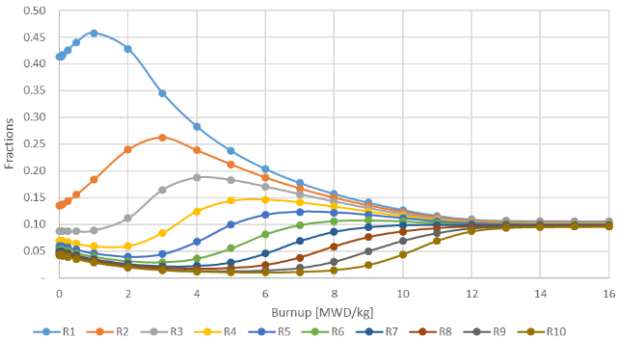

Figure 3. Atomic reaction rate fractions of Gd-155.

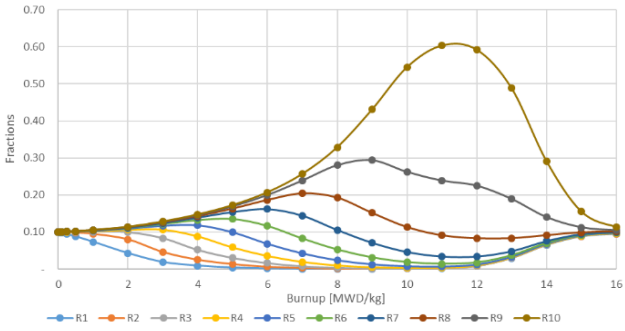

Figure 4. Quantity fractions of Gd-155.

Figure 5 is the plot of the change of homogeneous atomic reaction rate of Gd-155 in a pin. From 0 to 8 MWD/kg, the reaction rate change of Gd-155 appears to be linear, but **Figure 3** proved that the spatial variation is very severe. The drastic changes of atomic reaction rates in outer FXRs are smoothed by homogenization and its effect cannot be taken into account during calculation.

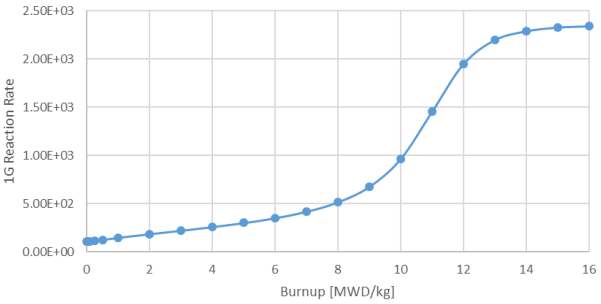

Figure 5. Homogenized atomic reaction rate of Gd-155.

From this observation, it is obvious that the effectiveness of the Gd quadratic depletion method is limited in homogeneous depletion. Since the quadratic function is fit to the smoothed reaction rate, it will only mitigate the time differencing error, not the heterogeneity effect. Thus to make the quadratic depletion method have full effect, it should be applied FXR-wise.

Consequently, the depletion calculation in the neutronics codes which employ pin-homogenized group constants require special treatments to handle these heterogeneity issues.

3. Heterogeneous Depletion Scheme

The main objective of the heterogeneous depletion scheme is to construct several Bateman equation systems per pin that take into account the heterogeneity explicitly, instead of a single homogenized system. In the following, the required quantities, detailed procedures to set the heterogeneous systems, and the solution scheme will be described.

3.1 Definition of Heterogeneous Quantities

To set up the heterogeneous depletion problem system, the following heterogeneous burnup matrix and number density vector should be defined:

$$\text{Burnup Matrix, } A_{ij,m} = \left\{ (\gamma_{ij}^{rct} - \delta_{ij})\sigma_{i,m}\phi_m + (\gamma_{ij}^{dec} - \delta_{ij})\lambda_i \right\} \Delta t$$

$$\text{Isotopic Number Density, } N_{i,m}$$

where i and j are the indices of nuclides, σ_i is one group microscopic cross section of which convert nuclide i to nuclide j, γ_{ij} is the yield fraction of i-th nuclide converting to j-th one from one reaction or decay and δ_{ij} is the Dirac-delta notation.

As the basic group constants and number densities are homogenized for a pin, the following additional constants should be generated from offline lattice calculations to obtain heterogeneous quantities:

Atomic Reaction Rate Fraction, $r_{i,m} \equiv \frac{(\sigma_i\phi)_m}{(\sigma_i\phi)_{tot}} = \frac{(\sigma_i\phi)_m}{\sum_m (\sigma_i\phi)_m}$

Atomic Quantity Fraction, $n_{i,m} \equiv \frac{N_{i,m}V_m}{\bar{N}_i V_{total}}$

Using these constants, the following heterogeneous reaction rates and the reduced number densities required to set-up the heterogeneous burnup matrices can be reconstructed from the pin-homogenized quantities:

Atomic Reaction Rate, $(\sigma_i\phi)_m = r_{i,m}(\sigma_i\phi)_{tot}$

Vol. Fraction Weighted Number Density, $N_{i,m} \equiv n_{i,m}\bar{N}_i$

3.2 Conservation Rules

To obtain the proper heterogeneous quantities with homogeneous variables, the quantities should satisfy the two conservation rules to be disscussed below. Two factors are required in these conservations rules: reaction rate fraction factor $\Gamma^k_{m,i}$, and microscopic cross section normalization factor $\tilde{\sigma}^k_i$.

For given atomic quantity fractions obtained from the solutions of heterogeneous depletion problems, these two factors are the solutions of two conservation equations. The fractions can be defined with below formula:

One conservation rule is the isotopic total reaction rate conservation for each FXR:

$$r^k_{m,i} n^k_{m,i} = \Gamma^k_{m,i}\left(N^k_{i,m}V_m\right)/\left(\bar{N}^k_i V_{tot}\right) \tag{3}$$

while the other is the isotopic total reaction rate conservation for the pin:

$$\bar{\sigma}^k_i = \sum_m \tilde{\sigma}^k_i \ \Gamma^k_{m,i}\left(N^k_{i,m}V_m\right)/\left(\bar{N}^k_i V_{tot}\right) \tag{4}$$

Note that, $\left(N^k_{i,m}V_m\right)/\left(\bar{N}^k_i V_{tot}\right)$ is not same as $n^k_{m,i}$. The number densities in the former are the solutions from pin-wise code, and the latter is from the lattice calculations. With above values gotten, we can get heterogeneous reaction rates like following formula:

Atomic Reaction Rate, $(\sigma\phi)^k_{i,m} = \tilde{\sigma}^k_i \Gamma^k_{m,i}\bar{\phi}^k$

The conservation rules in Eq. (3) can be questionable. Instead of using reaction rate fraction factor $\Gamma^k_{m,i}$, we can use to use atomic reaction rate fraction $r_{i,m}$ directly. However, the solutions of heterogeneous number densities can be different from the values from the lattice code. In that case, the conserved quantities need to be the total reaction rate which is more physically important, not the atomic reaction rate.

3.3 Heterogeneous Depletion Scheme

The above scheme follows the fully explicit time integration. As shown on it, the solution of heterogeneous depletion calculation should be re-homogenized at the end of every step.

In Figure 6, it is indicated that both homogeneous and heterogeneous depletions calculate the number densities of Gd isotopes. Although the homogeneous one updates the values on Gd isotopes, they will be overwritten with the heterogeneous solutions. Thus, it is possible to subtract Gd isotope chains from homogeneous calculations, unless the chains contain other nuclides. It will help to reduce computational costs.

$N^1_{m,i} = n^1_{m,i}\bar{N}^1_i$
DO k = 1, N_{steps}
  CALL SSEIG()
  (Hom. Depletion) $\bar{\mathbf{N}}^k = \exp\left(-\bar{\mathbf{A}}^k\Delta t^k\right)\bar{\mathbf{N}}^k$
  (Het. Burnup Matrix Construct) $\mathbf{A}^k_m = f\left(\Gamma^k_{m,i}, \tilde{\sigma}^k_i\right)$
  (Het. Depletion) $\mathbf{N}^{k+1}_m = \exp\left(-\mathbf{A}^k_m\Delta t^k\right)\mathbf{N}^k_m$
  (Re-homogenize) $\bar{N}^{k+1}_i = \sum_m N^k_{m,i}$
END DO
(i is the index of Gd isotopes)

Figure 6. Heterogeneous depletion scheme

4. Results

To assess the proposed heterogeneous depletion schemes, a single 2-D assembly problem, the B3 assembly type of APR-1400 reactor, was solved. At first, the number densities of Gd-155 and Gd-157 were compared. As they have the largest absorption cross section and error among Gd isotopes, two nuclides were the target. The variation of the two isotopes are shown in Figure 7 and 8.

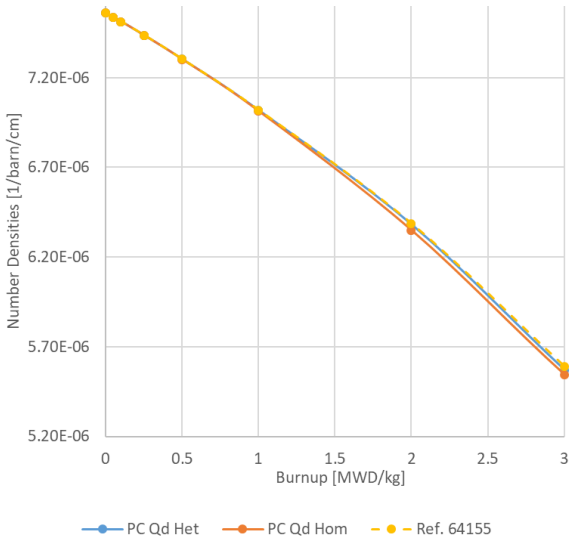

Figure 7. Gd-155 number density comparison.

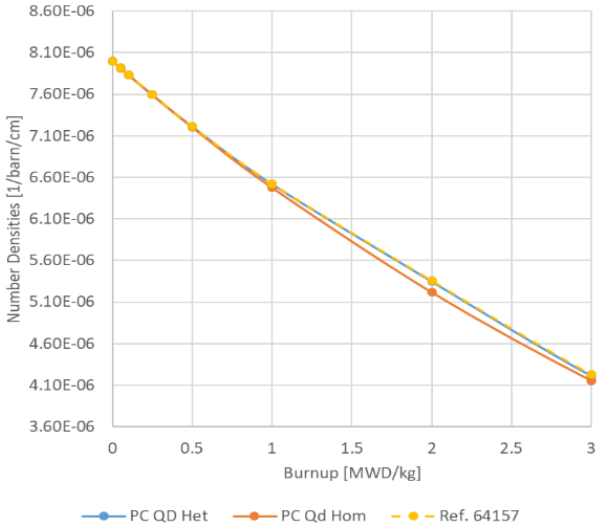

Figure 8. Gd-157 number density comparison.

The number density errors noted with the homogeneous scheme disappears with the heterogeneous scheme as shown in the two figures. The consequence of the reduced number density errors are shown in Figure 9 and 10 which show the multiplication factos and its error.

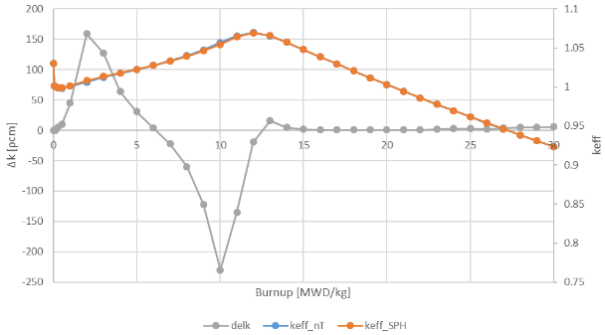

Figure 9. B3 SA k-eff with Homogeneous Scheme

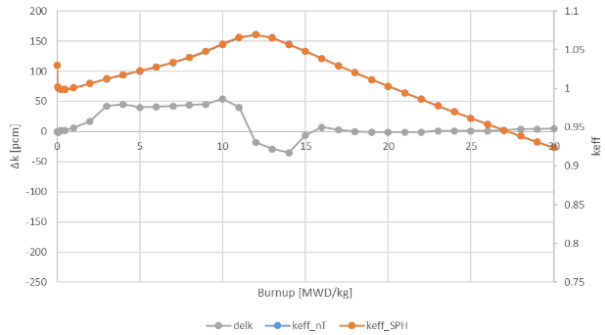

Figure 10. B3 SA k-eff with Heterogeneous Scheme

After 16 MWD/kg, two have no noticeable difference. Up to 15 MWD/kg, the result with heterogeneous scheme shows obvious better accuracy. Fluctuating errors on homogeneous depletion calculation are stabilized.

Finally, the power distribution at 10MWD/kg where the maximum relative error occurs is assesed. The error was the heterogeneous scheme is only 0.149 % even on Gd pins as shown in **Figure 11**.

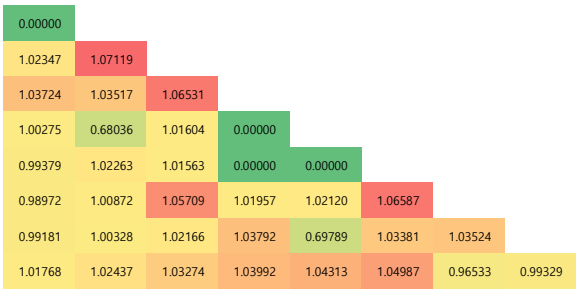

Figure 11. Calculated Power Distribution @ 10 MWD/kg

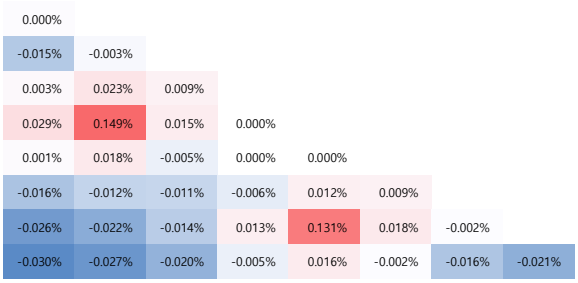

Figure 12. Power Distribution Error @ 10 MWD/kg

5. Conclusion

In this paper, the problems of the depletion calculation with pin homogenized quantities were explained and the heterogeneous solution scheme was proposed. With several result comparisons between the conventional scheme and proposed scheme, the effectiveness of heterogeneous depletion was proved.

The proposal of this new method is important. But what is more important is the discrepancy contained in the homogenized depletion problems. This issue has not been the matter in two step procedures. This should not be ignored as demonstrated in this work.

References

[1] H. H. Cho et al., "Preliminary Development of Simplified P_3 based Pin-by-pin Core Simulator, SPHINCS," Transactions of the Korean Nuclear Society Spring Meeting, Jeju, Korea, May 23-24.

[2] Y. S. Jung, C. B. Shim, C. H. Lim and H. G. Joo, Practical Numerical Reactor Employing Direct Whole Core Neutron Transport and Subchannel thermal/hydraulic Solvers, Annals of Nuclear Energy, Vol. 62, p.357-374, 2013.

[3] A. Yamamoto, Y. Kitamura and Y. Yamane, Cell homogenization methods for pin-by-pin core calculations tested in slab geometry, Annals of Nuclear Energy, Vol. 31, p.825-847, 2004.

[4] Jiwon Choe et al., Analysis of Effective Gd Depletion Model, Transactions of the Korean Nuclear Society Spring Meeting, Jeju, Korea, May 17-18.

[5] Z. WEISS, A Consistent Definition of the Number Density of Pseudo-isotopes, Ann. Nucl. Energy, Vol. 17, pp. 153-156, 1990.

[6] D. Lee et al., Quadratic Depletion Model for Gd Isotopes in CASMO-5, Advances in Nuclear Fuel Management IV, LaGrange Park, IL, USA, April 12-15, 2009.