Spectral History Correction of Microscopic Cross Sections for the PBR Using the Slowing Down Balance

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Abstract

A method has been formulated to account for depletion effects on microscopic cross sections within a Pebble Bed Reactor (PBR) spectral zone without resorting to calls to the spectrum (cross section generation) code or relying upon table interpolation between data at different values of burnup. In this method, infinite medium microscopic cross sections, fine group fission spectra, and modulation factors are pre-computed at selected isotopic states. This fine group information is used with the local spectral zone nuclide densities to generate new cross sections for each spectral zone. The local spectrum used to generate these microscopic cross sections is estimated through the solution to the cell-homogenized, infinite medium slowing down balance equation during the flux calculation. This technique is known as Spectral History Correction (SHC), and it is formulated to specifically account for burnup within a spectral zone.

It was found that the SHC technique accurately calculates local broad group microscopic cross sections with local burnup information. Good agreement is obtained with cross sections generated directly by the cross section generator. Encouraging results include improvement in the converged fuel cycle eigenvalue, the power peaking factor, and the flux. It was also found that the method compared favorably to the benchmark problem in terms of the computational speed.

KEYWORDS: Pebble Bed Reactor, PEBBED, cross section, spectral history, spectrum, burnup

1. Introduction

The PBR fuel cycle code PEBBED [1] under development at the Idaho National Laboratory (INL) solves for the steady-state burnup and flux distributions in the PBR using integrated diffusion and depletion solvers and a unique approach to coupling them to the pebble flow [2]. The lack of *a priori* knowledge of the asymptotic fuel cycle nuclide composition requires that microscopic cross sections be regularly interpolated from tables or generated directly from a spectrum code during the core simulation computations. Cross sections generated for a batch of pebbles in one location or at a given step during the iterative process may not be valid for other locations or at later iterations.

A PEBBED simulation is initialized with a single broad group microscopic cross section library applied to the entire reactor. This cross section library is generated with an assumption regarding the isotopics of a converged equilibrium fuel cycle solution. Generally, the nuclide

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distribution corresponding to a core-averaged burnup of a converged equilibrium cycle is used to create this initial library. However, the spectrum corresponding to this equilibrium cycle is unknown initially, meaning that the assumptions regarding this initial cross section library are inaccurate.

Currently, the cross section methodology in use by PEBBED involves dividing the PBR reactor, including the flowing fuel-and-graphite pebbles and the graphite reflectors, into spectral zones. A spectral zone is a collection of meshes over which the spectrum is assumed to be relatively static. In its present form, PEBBED addresses cross section updates through iteration on several fuel cycle simulations. There are also two other possible approaches for cross section treatment in PEBBED, interpolation from pre-computed cross section libraries, or online calls to a spectrum code such as COMBINE [3] or MICROX-2 [4]. In the interpolation approach, burnup dependent cross section libraries could be pre-computed for many depletion states. During the course of the simulation, the average burnup of a zone would be computed and the closest possible cross section library extracted for that state. In the iteration approach, the simulation is started at an average burnup level, an asymptotic solution is found, and the densities corresponding to that solution are used to construct new cross section libraries with the spectrum code. These libraries are used to start a new PEBBED simulation to a new asymptotic solution, and the process is repeated until convergence.

All three approaches have limitations. The difficulty with the iteration approach is that there is no mechanism for updating the cross sections during the course of the solution, as these are used in the flux and burnup calculations. The interpolation approach, while fast, requires that an enormous library of data be generated to encompass the expected spectral domain. The third approach, direct calls to a spectrum code, provides the most accurate results but is computationally demanding when large numbers of spectral zones are used, or when several fuel cycle simulations are completed to find an optimum fuel cycle.

A new method is proposed by which an infinite medium microscopic fine group cross section library is pre-computed at different isotopic states then coupled with local nuclide densities to generate appropriate local cross sections. The infinite medium slowing down balance equation is solved using these local cross sections for a local spectrum calculation.

PEBBED converges to an equilibrium fuel cycle through the use of three burnup iteration loops. The outer loop checks that the discharge burnup target is met (generally 80 to 95 MWD/kg). The second loop iterates upon the entry plane burnup (or nuclides mix), which depends upon the discharged fuel recirculation methodology. The entry plane nuclide densities are coupled to the discharged nuclide densities through a recirculation matrix [2]. The third, inner burnup loop converges upon the cell-wise burnup and flux distribution.

Within the inner burnup loop, the updated nuclide densities in a node (or sub-zone), due to the depletion calculation, are used to construct the macroscopic cross section for the flux solver as,

$$\Sigma_{x,h}^{(n)} = \sum_i \bar{\sigma}_{x,h}^{i,(n)} N^{i,(n)} . \qquad (1)$$

In Eq. (1), the symbols "(*n*)", "*x*", "*h*", and "*i*" refer to the isotopic state, reaction type, broad group number, and the isotope, respectively. A bar over a quantity in this study indicates that it has been averaged over an entire spectral zone. In Eq. (1), the microscopic cross section library has been averaged over the spectral zone. PEBBED solves the coupled depletion/diffusion equations to determine the updated isotopic densities in each node. The new atomic densities $N^{i,(n+1)}$ are used to recalculate the updated macroscopic cross sections, $\Sigma_{x,h}^{(n+1)}$ for another diffusion calculation. The following approximation is made.

$$\Sigma_{x,h}^{(n+1)} \cong \sum_i \bar{\sigma}_{x,h}^{i,(n)} N^{i,(n+1)} \tag{2}$$

This is repeated until the burnup distribution in the core converges.

However, with the change in entry plane burnup due to pebble discharge, and upon entering the inner burnup loop again, it is necessary to update the microscopic cross section library such that its state (n) is as close as possible to state (n+1). In order to update the microscopic cross section library at (n) such that it reflects the isotopic changes within a spectral zone as closely as possible, a new fine group spectrum at (n) is calculated for that spectral zone.

The approach of spectral history correction is to extend the applicability of a master set of fine group cross section libraries to a wide range of local isotopic conditions. The method circumvents calls to the spectrum generation code and avoids cross section interpolation during the simulation. The fine group flux spectrum needed to collapse $\bar{\sigma}_{x,h}^{i,(n)}$ for isotopic changes within each spectral zone is estimated through the solution to the infinite medium slowing down balance. Each spectral zone has a unique cross section library that is recalculated by SHC in the PEBBED simulation. The combined diffusion-depletion-spectrum generation process is repeated until the solution converges to a self-consistent core burnup and flux state.

The chief supposition of the burnup correction method developed in this study is that, due to the linearization of the decay chains in PEBBED, it is possible to track the isotopics of the pre-computed fine group libraries in terms of the U-235 density of the spectral zone.

2. The Method: Spectral History Correction

2.1 Infinite Medium Slowing Down Balance

The idea behind this method is that the new fine group spectrum required for the update in Eq. (2) may be obtained from the solution of the infinite medium slowing down balance in each spectral zone with the PEBBED updated atom densities. The balance equation in the multigroup form is given as,

$$\sum_{i=1}^{N}\left[\bar{\sigma}_{t,g}^{i,(n)}\bar{N}^{i,(n+1)}\right]\bar{\Phi}_{g,\mathrm{hom}}^{(n+1)} = \sum_{g'=1}^{G}\sum_{i=1}^{N}\left[\bar{\sigma}_{s,g'\to g}^{i,(n)}\bar{N}^{i,(n+1)}\right]\bar{\Phi}_{g',\mathrm{hom}}^{(n+1)} + \frac{\bar{\chi}_g^{(n)}}{k_\infty}\sum_{g'=1}^{G}\sum_{i=1}^{N}\left[\nu\bar{\sigma}_{f,g'}^{(n)}\bar{N}^{(n+1)}\right]\bar{\Phi}_{g',\mathrm{hom}}^{(n+1)}. \tag{3}$$

From Eq. (3), it can be seen that the microscopic cross sections at the n^{th} state are combined with the nuclide densities at the $(n+1)^{\mathrm{th}}$ state in the slowing down balance. The updated nuclide density, $\bar{N}^{i,(n+1)}$, is the result of averaging the cell wise nuclide density over the spectral zone.

The ratio of the homogeneous to the heterogeneous spectra is pre-computed by the spectrum code and stored with the libraries at each isotopic state (n). This ratio, denoted the fine group modulation factor, is applied to correct the homogeneous calculation for heterogeneous effects in SHC. With the ratio of the homogeneous to heterogeneous solution from the fine group libraries defined as,

$$\mu_g^{(n)} = \bar{\Phi}_{g,\mathrm{hom}}^{(n)} / \bar{\Phi}_{g,\mathrm{het}}^{(n)}, \tag{4}$$

the homogeneous flux solution from the solution of Eq. (3) may be corrected in the following manner.

$$\bar{\Phi}_{g,SHC}^{(n+1)} \cong \bar{\Phi}_g^{(n+1)} / \mu_g^{(n)} \tag{5}$$

The new coarse-group microscopic cross sections are then estimated with Eq. (2) using the flux solution from Eq. (3) as,

$$\bar{\sigma}_{x,h}^{i,(n+1)} \cong \sum_{g\in h} \bar{\sigma}_{x,g}^{i,(n)} \bar{\Phi}_{g,SHC}^{(n+1)} \Big/ \sum_{g\in h} \bar{\Phi}_{g,SHC}^{(n+1)} . \quad (6)$$

The transport cross section is collapsed with an estimate of the current [4].

2.2. The Fine Group Libraries

Microscopic cross section libraries are pre-computed for sets of representative spectral zone-averaged nuclide densities. These nuclide densities are based upon edits from a PEBBED simulation of a Pebble Bed Modular Reactor, Dynamic Inner Reflector (PBMR-DIR) design [5], to be described in Section 3.2. Stored with the cross sections was the fine group fission spectrum for the mixture and the fine group modulation factor. These libraries were generated using the NJOY/MICROR/MICROX-2 system [6], [7], [4]. The 141 group fine structure is a subset of the General Atomics group structure [4].

These libraries were tracked in terms of the spectral-zone averaged U-235 density. Because of the linearization of the decay chains in PEBBED, it is possible to track a zone-average mixture in terms of the density of U-235.

3. Implementation and Results

3.1. SHC Implementation

The re-computation of the cross sections for depletion effects within the spectral zone was accomplished through the solution of the infinite medium slowing down balance (Eq. (3)) within each spectral zone of the fuel core. This technique was implemented in PEBBED by replacing the existing table lookup with a subroutine to which the nuclide data was passed. This subroutine, named SHC, recalculated the microscopic cross sections with the most recent nuclide densities. All calculations were performed at a core-averaged PBR operating temperature of 1073 K.

Two update methods were employed to generate cross sections: the direct update in which MICROX-2 was called to compute cross sections, and the spectral history update in which the cross sections were computed with the SHC method. The direct update method served as the benchmark for the SHC method.

As a measure of improvement, a base case with no cross section update was performed. This case is denoted the Uncorrected Case (UC). In this case, the initial cross section library was used throughout the simulation.

All PEBBED models were initiated with the same infinite medium, approximate core-averaged mid-burnup (~ 45 MWD/kg) isotopic cross section library at six broad groups. For the benchmark and SHC cases, however, the cross sections were recalculated for each spectral zone with each entry plane burnup iterate.

The benchmark problem involved system calls by PEBBED to MICROX-2 with local spectral zone averaged nuclide densities as arguments; MICROX-2 was run as an infinite medium problem to capture burnup effects for this benchmark.

The microscopic cross sections which are tracked by PEBBED and which are recalculated by SHC include the scattering matrix, the transport cross section, the absorption cross section, nu-fission, and the fission cross section, all per nuclide. These cross sections were recalculated for all nuclides currently tracked in PEBBED. The broad group energy structure that was used in the PEBBED simulations was a variant of the V.S.O.P. structure [8] with the

addition of a thermal boundary at 2.38 eV.

3.2. The PBR Model

The PBR example (test problem) was formulated to quantify the extent of the change in the spectral zone isotopics, due to both pebble recirculation and pebble burnup, upon certain converged PBR core parameters. The PBR design chosen for testing was a variation of the PBMR-DIR theme originally proposed as a prototype by PBMR Ltd. The considered design for this study was later adapted and improved at the INL for use with PEBBED pebble bed reactor design optimization studies [5].

Regarding model specifics, the core thermal power of this reactor design is rated at a constant 268 MWth of power. The flow rate is 5140 core pebbles per day. The ex-core decay time for the fuel pebble is 5 hours.

The basic configuration of this reactor type is that of two major zones, a moving cylindrical inner reflector of graphite pebbles, and an outer annulus of fuel pebbles. Both pebble types move down through the core, being discharged from an output cone and reloaded into the top. In the case of continuous refueling, discharged, partially burned fuel pebbles are reloaded into the top of the core, along with fresh fuel pebbles. In the case of graphite moderator pebbles, the loading is achieved by means of a centrally located tube. Fuel pebbles are loaded through radially spaced tubes from the reactor center. To achieve greater fuel economy, the fuel pebbles are burned to a very high burnup (80 MWD/kg-U) and consequently discharged. Thus, the core was considered to be a recirculating core and modeled as such, meaning that, discharged pebbles that don't reach the target burnup are reloaded with fresh pebbles. In this design, 75 % of the core total pebble flow is in the outer fuel zone annulus.

This PEBBED model incorporates five flow channels for the flowing part of the core: channels one through two correspond to graphite pebbles and channels two to five contain fuel pebbles. The channels are evenly divided such that the flow fraction for each channel is approximately ~0.20. The second channel includes both graphite and fuel pebbles. This second channel is known as the mixing zone of the core. In the PBR design considered for this study, the fuel pebble loading distribution is neither burnup nor pass dependent (pass denoting the number of times the pebble traverses through the core, 10). The consequence of the independent burnup distribution is that all burnup stages of the pebbles are represented equally in the considered spectral zones in the converged fuel cycle solution. The simulations were two-dimensional, encompassing half of a cylindrical core with 30 cells in the positive radial direction, 88 cells in the positive axial direction. In the radial direction, the inner boundary condition is that of zero current, and the outer boundary condition is that of zero flux. Zero current boundary conditions exist at the top and bottom of the reactor in the axial direction.

The general shape of this reactor design is of four reflectors that surround an inner core of downward flowing fuel pebbles. Three of the reflectors are of graphite bricks and they are situated at the top, bottom and on the radial side. The inner reflector consists of flowing graphite pebbles. In this study, only the cross section libraries corresponding to the flowing pebble core were updated (the graphite pebbles, the graphite-fuel mixture zone, and fuel pebbles). Table 1 indicates some of the dimensions of the PBMR-DIR in (cm).

In this PEBBED model the cell nuclide densities are homogenized over a Body Centered Cubic (BCC) lattice arrangement. For the benchmark problem, the Dancoff factor was recalculated from coded analytic formulae at each cross section update [9]. This was to ensure consistency between the Dancoff and the actual outer layer graphite density obtained in the moderator region.

In the simulation, the core is initially loaded with fresh fuel pebbles and graphite pebbles.

Table 1: PBMR-DIR Model Dimensions [cm].

Top Reflector	Radius = 250; Height = 135
Gas Plenum	Height = 20; Width = 96.25
Pebble Core	Radius = 175; Height = 850
Radial Reflector	Radius = 75; Height = 850
Bottom Reflector	Radius = 250; Height = 260

3.3. Results

The results of the implementation are presented in Table 2. In order to get a relative idea of the improvements in the method, in addition to SHC being compared to the benchmark case, the uncorrected XS case was also compared to the benchmark case.

The terms of comparison from the converged equilibrium pebble bed core are the eigenvalue, the power peaking factor, the flux % root mean square (RMS), and the fission density % RMS. A postprocessor code was written to read the PEBBED output and to calculate these errors. The flux % RMS error considered was the one group flux calculated per mesh cell, summed over that portion of the reactor consisting of flowing pebbles.

The fission density is defined over the fuel zone of the core as,

$$(I \cdot J) \cdot \Sigma_f(i,j) \cdot \Phi(i,j) / \sum_{i=1}^{I} \sum_{j=1}^{J} \Sigma_f(i,j) \cdot \Phi(i,j) . \quad (7)$$

Both the SHC and uncorrected models are compared to the benchmark.

Table 2: Spectral History Correction (SHC) and Uncorrected (UC) Methods vs. Benchmark. Method.

	Local cross sections from MICROX (Benchmark)	**Global cross sections only (UC)**	**Error**	**SHC-generated local cross sections**	**Error**
Eigenvalue	*1.0380192*	*1.0409036*	*2.884* [(a)]	*1.0376886*	*-0.3306* [(a)]
Max. PPF	*1.69*	*1.65*	*-2.37* [(b)]	*1.69*	*0.00* [(b)]
Mean PPF	*1.57*	*1.53*	*-2.55* [(b)]	*1.57*	*0.00* [(b)]
	SHC % RMS Error			**UC Relative % RMS Error**	
Flux	*5.33E-03*			*5.32E-02*	
Fission Density	*5.04E-03*			*1.25E-01*	

[(a)] in units of mk; [(b)] relative error

3.4. Discussion

The use of the SHC algorithm with PEBBED led to considerable improvement in

predicting the core equilibrium eigenvalue. The PEBBED/SHC combination only under-predicted the converged core eigenvalue by about ~ -0.33 mk, as compared to the benchmark, whereas the uncorrected case (UC) over-predicted the core equilibrium eigenvalue by almost ~2.9 mk. This is almost a factor of 9 improvement in the neutron balance of the converged core. The relative error for SHC for the maximum power peaking factor (PPF) and mean power peaking factors is 0.0 %, which is excellent. This presents a drastic improvement over the error presented by the uncorrected case (UC) of ~-2.4 % and ~-2.6 % for the maximum and mean power peaking factors. The fission density improved by nearly a factor 24, and the one group flux improvement was almost 10 fold.

A call to SHC at the beginning of the cycle for one spectral zone took approximately ~ 0.96 seconds, while a call to the MICROX benchmark for the same spectral zone (which included density and Dancoff factor calculations and file handling) was clocked at ~ 1.7 seconds.

4. Conclusions and Future Work

A spectral history method to correct microscopic cross sections for the change in isotopics due to fuel burnup and pebble recirculation is developed with excellent results. The SHC method depends upon the computation of unique fine group spectra in specific zones of the PBR core. A set of fine group microscopic cross section libraries, fission spectra, and flux modulation factors is computed by the cross section generator and tracked in terms of the U-235 density.

Future work includes applying SHC to different PBR configurations and models and more importantly extending the method to account for the effect of neutron leakage on the cross sections. No attempt was made to optimize cross section data handling and therefore the efficiency of the SHC module. For example, the development of a binary form of storage for the cross section libraries is expected to improve the computational speed of the method.

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