THE CORRECTION OF PEBBLE BED REACTOR NODAL CROSS SECTIONS FOR THE EFFECTS OF LEAKAGE AND DEPLETION HISTORY

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

SUMMARY

An accurate and fast method is presented to generate nodal cross sections for the Pebble Bed Reactor (PBR). This method takes into account the current isotopics (depletion state) in the node, along with the leakage patterns to and from the node. This method relies upon the numerical solution to the slowing down problem with homogeneous macroscopic cross sections. These cross sections are constructed on the basis of a pre-computed microscopic cross section library, parameterized in terms of fuel isotopic densities, and combined with spectral-zone averaged atom densities. With this assumption for the construction of the macroscopic cross sections, a fine multigroup spectrum can be solved for on the basis of B_1 slowing down theory. With this new spectrum, the microscopic cross section library may be recollapsed in energy to the broad group structure employed by the fuel cycle code. The result is a fast method that compares favorably to the benchmark scheme of calculation with the lattice cross-section generator.

The node, in a general sense, is referred to as a spectral zone in this work, and it indicates that part of the flowing reactor core in which the spectrum is assumed to be approximately non-varying. In the recirculating PBR core, a tall reactor vessel contains spherical fuel elements that move downward through the core during operation. Each element drops out of the core and is reloaded until it achieves a specified discharge burnup. Thus, any local region of the core consists of a random collection of pebbles at various burnup stages. The double heterogeneity of the fuel and the indeterminate

burnup and geometry of the spectral zone poses a unique challenge for the computation of local cross sections.

After a sufficiently long period of continuous refueling and operation, the PBR reaches a steady state in which the isotopics and the average burnup remain constant. This steady state is known as the equilibrium cycle. Considerable neutron leakage between spectral zones, along with the initial lack of knowledge of zone nuclide composition and leakage patterns requires that cross sections must be repeatedly recomputed during the core simulation to the steady state fuel cycle. The current methodology for treating these cross sections entails two approaches: extensive tabulations as functions of key parameters or repeated calls to the spectrum code during the core simulation. The latter is the most accurate but can be computationally expensive.

An alternative technique, known as Spectral History Correction (SHC), has been formulated to compute the local microscopic cross sections within each spectral zone with information from the core simulation. In SHC, a set of fine group libraries pre-computed at specified depletion and relative moderation states is coupled with the local spectral zone nuclide densities and group bucklings to re-compute a new spectrum for each spectral zone. The relevant fine group cross-section library is then recollapsed to the local broad group cross-section library.

CHAPTER 1

INTRODUCTION

There are two main issues governing the modeling of the neutron population within the fuel portion of a nuclear reactor core: the determination of the distribution of neutrons in position, energy, and direction; and the calculation of physically accurate neutron-nuclear interaction cross-sections. This work addresses the second issue. Broadly, the cross section may be characterized as the probability for the occurrence of a particular reaction type at a certain position and energy. This probability is often expressed per nuclide, as a microscopic quantity, or per mixture, as a macroscopic quantity. The macroscopic cross-section, conveying the interaction probability of a neutron with a group of nuclides in a material, comprises the main physical set of constants for the Boltzman transport equation.

These cross section data are the chief input to the discretized Boltzman equation for the neutron balance in a reactor. In core analysis, it is necessary to homogenize these cross sections in space and in energy. In space, core design often calls for complex arrangements of fuel and moderator, structure, and coolant to fulfill economic constraints and to satisfy safety considerations. Thus, the cross section is smeared, or homogenized for representative portions of the spatial domain as a way to preserve computational economy. In energy, the actual physical behavior of the cross section can be quite complex owing to the high interaction probabilities of the neutron with a heavy metal target nucleus at specific quantum states. These high probabilities, known as the resonances, characterize the energy dependence of the target nuclide under bombardment

by a neutron. When viewed in experimental form, the structure of the resonances is very detailed. These are calculated per target nuclide by scientific measurements, with gaps in the data being filled with theoretical predictions. At the reactor lattice level (a repeating arrangement of fuel, moderator, and coolant), the microscopic cross section is weighted with the nuclide number density in the lattice to form the macroscopic cross section, which feeds into the transport equation for solution of a flux distribution. The calculation of macroscopic cross-sections that enforce neutron balance, preserve nuclear reaction rates and the core eigenvalue, and preserve the pointwise resonance structure is thus a daunting and expensive task.

The averaging of the cross section over energy is in itself an involved process that entails the solution of a simplified form of the Boltzman transport equation for a weighting function. Ordinarily, to concentrate on the energy dependence of the flux, a simple spatial mode is assumed; rigorously, this is equivalent to Fourier transforming the transport equation. This spatial mode, known in reactor physics as the buckling, describes the relative spatial gradient of the neutron flux. With this buckling definition, a simplified transport equation is derived. In this form, this equation describes the energy dependence of the flux, known as the spectrum.

The detailed solution for the spectrum is usually discretized over a great number of energy points or groups and solved over this fine grid. The solution for the weighting function is completed in a pointwise manner. With this weighting function, the pointwise cross section is averaged over a defined energy decrement. This energy width, known as a group, usually corresponds to physical considerations of the relative energy between the

neutron and the nuclide. The averaging over the group is completed such that specific groupwise nuclear reaction rates are conserved.

In the analysis of the Light Water Reactor (LWR) type in widespread commercial use, this solution is completed for a repeating lattice of fuel and moderator with idealized boundary conditions. The fuel contains the fissile and fertile nuclides that consist of the heavy metals which fission to give neutrons. The moderator of the lattice contains light nuclides (such as water for the LWR), which slow down the born fast neutron to an energy at which it can be absorbed into the fuel for another fission reaction. The coolant keeps the fuel from melting due to the fission heat and is also water in the LWR. In the standard LWR methodology, the macroscopic cross sections, known as the group constants, must be re-calculated many times, and between calculations the determination of the group constants depends heavily upon parameterizations in terms of variables such as the fuel and moderator temperature, the fuel exposure, and the neutron poison concentration. A great deal of research has been done with the maturation of the nuclear power industry into the proper manner to generate cross sections for LWR's, with the consequence that there are a variety of approaches to this problem.

The Pebble Bed Reactor (PBR) is presently the subject of research worldwide as an improvement over the conventional LWR type. One of the design candidates as part of the Generation IV Nuclear Energy Initiative, the PBR offers several advantages over the LWR type including passively safe design and higher operating temperature (for secondary industrial heat), and proliferation resistance. However, aside from the pros, the PBR presents unique modeling difficulties in terms of analyzing the fuel cycle and in generating the cross sections. In the PBR, the lattice consists of a spherical fuel element

encased in a graphite shell. The fuel element itself is filled with heavy metal fuel grains coated with layers of silicon and carbon to retain fission products. These grains are suspended in a graphite matrix. Graphite serves as both the moderator and the structural material in the PBR. The PBR coolant is helium (as opposed to the water-cooled LWR). One of the unique features of the PBR is that the elements move downward through a tall reactor vessel, accruing burnup in the core. Because of the spherical shape of the fuel elements and their movement through the core, distinctive difficulties are presented in terms of cross section generation.

Allowing for the complexity of repeatedly finding group constants in the LWR fuel cycle, an accurate characterization of the cross section in the Pebble Bed Reactor is considerably complicated by the various levels of heterogeneity (at the grain and pebble levels), the spherical shape of the fuel elements, the movement of the fuel, and the randomness of the grain and pebble distributions in the core. On top of this undertaking, the PBR fuel cycle code being improved by this method reaches an equilibrium fuel cycle solution without the beforehand knowledge of the converged nuclide, flux, and power distributions. In addition to this lack of initial information the convergence path to the equilibrium fuel cycle is also unknown.

As the cross sections characterize the probability for certain classes of interactions, their accurate determination is important for the neutron economy during the flux and depletion calculations. However, with the paucity of data regarding the converged solution, it is difficult to define an initial cross section library that will remain valid throughout the calculation without an update of that library. It is also difficult to propose a master library for all burnup and leakage states that might be present in the

reactor as these are simply not known. Thus, the problem lies in the most efficient manner to recalculate the cross section library such that it reflects the most current operating conditions. The ideal situation would be a cross section library constructed instantaneously with the actual leakage and burnup patterns present in the core, both on the path to convergence and for the equilibrium state. However, the spectrum, in the pre-equilibrium states and in the equilibrium solution, is not initially known, hence the difficulty in producing accurate cross section data to start the fuel cycle analysis. This problem is compounded when optimization studies are undertaken. Then, it is possible to run many fuel cycle simulations to seek an optimum subject to certain constraints, and it would be even more difficult to characterize what the spectrum would be at this optimized equilibrium cycle.

CHAPTER 2

LITERATURE REVIEW

Diffusion nodal methods are an established analysis tool for the design and monitoring of the conventional Light Water Reactor (LWR) cores of today. Fluxes and currents are averaged over the volume and surface of a cell such that reaction rates and surface leakages are conserved, and a coarse mesh diffusion equation is solved with representative nodal cross sections. To save on computational economy, the depletion calculation is ordinarily completed for a single fuel assembly with simplified boundary conditions.

In the LWR, the spectral effects upon the cross sections arise from the presence of neighboring assemblies and control blades. The effect of the neighboring nodes upon the assembly is accounted for through several approaches, among them table look-up and interpolation, boundary perturbation methods, empirical correlations, and semi-analytical methods. However, in the Pebble Bed Reactor (PBR), spectral effects arise primarily from the burnup of neighboring spectral zones, which are then coupled to the zone of interest through energy dependent leakages.

2.1. Light Water Reactor Cross Section Methodology

In the Light Water Reactor, the influence of the spectral effect upon the spatial dependence of the nodal cross section has been researched extensively. Ordinarily, the fuel composition change is calculated at the pin-cell level in a single fuel assembly with idealized (reflective) boundary conditions that may not capture neighboring assembly environmental and depletion effects (Forslund et al., 2001). After the fuel change and fission product buildup are calculated with a lattice depletion code, the critical control position (in the case of the Boiling Water Reactor) and flux distribution are recalculated. This procedure is repeated as the assembly is depleted, with a consequent back-and-forth recalculation of the flux and control rod (CR) position; it is then necessary to recalculate the cross sections at each depletion step either through re-computation or interpolation from tables (Stacey, 2001). The group constants must be regenerated through the fuel cycle hundreds of times, and these group constant recalculations can lead to great expense in nodal diffusion analysis.

In order to avoid expensive recalculations, extensive parameterizations in the fast, resonance, and thermal regions of the neutron spectrum are normally performed (Duderstadt and Hamilton, 1976). This leads to the construction of tables of cross sections (macroscopic and microscopic) at many values for these parameters. Interpolation is then used to approximate the information between data points. This approach has been relatively successful for LWR's since the cross sections can vary smoothly with "independent" variables of the parameterizations. In the fast spectrum, the parameter of most interest is the moderator-to-fuel density ratio in the homogenized

lattice, whereas in the thermal region the parameterization is carried out as functions of both the temperature and the absorption to scatter ratio. In the resonance spectral region, the modeling is more difficult, with several parameters being used to define the resonance integrals.

Outside of considerations for the specific node burnup and exposure, the time behavior of the reactor environment is difficult to model when considering the spectral effects of neighboring nodes. That is, aside from the desire to deplete the assembly at the most correct core environment conditions, the previous state of the node can influence its current isotopics. The spectral history effect is then defined as the effect of the change in the fast-to-thermal flux ratio with fuel burnup upon the U-235 fission, coupled with the effect of fission product buildup.

In the case of the Pressurized Water Reactor (PWR), the spectral effects are due primarily to operating conditions such as the exposure, the moderator density, and the boron concentration. Burnable poisons in one part of the cycle influence the isotopics in the next part, even when the poisons are absent in the next part of the cycle. This phenomenon, known as the density effect, is felt when a node is depleted at core-averaged moderator conditions; due to the PWR axial temperature gradient, the use of a core-averaged density leads to employing under-moderation at the bottom of the core and over-moderation at the top of the core. The macroscopic cross sections for each axial spectral zone are generated with a core averaged moderator density and with a spectrum averaged over the spectral zone, the level of accuracy in the cross sections depending upon the number of spectral zones considered. Spectral history effects are normally taken into account either through the use of detailed microscopic cross section tables with

all fertile and fissile nuclides with fission products, or with parameterization of a pseudo-macroscopic cross section as functions of exposure (DiGiovine and Smith, 1995). Several studies have found significant PWR spectral effects in regard to axial flux shift and core reactivity (DiGiovine and Smith, 1995; Gavin, 1995). The conclusion for PWR analysis was that the nodal cross sections depend not only upon the local exposure but also on the local conditions at which depletion occurred.

However, the spectral history problem isn't as severe in the PWR as in the BWR. While in the BWR the spectral history effects are induced both by control rod insertion and a spectral mismatch between assemblies, most of the spectral history effects are due to insertion of the control blades (Iwamoto and Yamamoto, 1999). The control blade suppresses the depletion of fissile fuel in the vicinity of the control blade and leads to a retention of the initial excess reactivity while additional excess reactivity may build up from conversion of U-238 to Pu-239, with the result of Pu-239 accumulation near the control blade.

Ordinarily in the BWR cross-section methodology, the spectral effect is accounted for in several ways: polynomial expansions of the nodal parameters in terms of such variables as the spectral history, temperature, nuclide densities, and nodal exposure (Iwamoto and Yamamoto, 1999); interpolation with and without a control blade, for example (Sitaraman and Rahnema, 1993); parameterizations of the nodal parameters (Garcia-Herranz et al., 1999), (Baturin and Vygovskii, 2001); through semi-analytic methods (Lee et al., 1996); or through boundary condition perturbation methods (Rahnema and McKinley, 2002).

For core-level coupled neutronic/thermal hydraulics simulations, cross section tabulations can become quite extensive, with the cross section being parameterized from such things as the fuel burnup, control variables, and the thermal hydraulics (Watson and Ivanov, 2002). To deal with off-nominal transients, and to decrease the number of data points required, such as in the case of the nonlinear behavior of the cross sections, it is necessary to use several variables to fix the thermodynamic state of the moderator/coolant, and to employ spline interpolation over the surface defined by these tabulations. The boundaries of this region are set such that interpolation can be done from the boundaries.

2.2. The Pebble Bed Reactor

The Pebble Bed Reactor (PBR) is one of several leading reactor types being considered as part of the Generation IV Nuclear Energy Initiative (Magwood, 2001). It offers several advantages over the conventional Light Water Reactor (LWR) type including passively safe engineering design, higher operating temperature (for hydrogen production and secondary industrial heat), and proliferation resistance (Terry et al., 2002). However, the PBR presents modeling challenges for fuel cycle analysis. The PBR belongs to a larger class of reactors named High Temperature Reactors (HTR's), which denote those reactors that are graphite moderated, gas cooled, and have high temperature operation. The other example of HTR is the type made with prismatic fuel, in which the fuel pellets are encased in large hexagonal graphite blocks, some examples including the Dragon Project in the United Kingdom, the Peach Bottom reactor near

Pittsburgh, and the prismatic reactor located at Fort St. Vrain near Denver (Massimo, 1976).

The pebble bed reactor concept is well described in the literature (Zhong and Qin, 2001; Schulten, 1978; Frewer et al., 1985). Perhaps the first pebble reactor that is closest to the present day designs was the experimental AVR of the Federal Republic of Germany (Schulten, 1989), which operated as a test reactor for twenty-five years. Germany also constructed the thorium cycle, pebble bed reactor, the THTR-300, which ran safely for five years (Dietrich and Roehl, 1996). At the Paul Scherrer Institut in Switzerland (PSI), a Pebble Bed Reactor, named PROTEUS, was extensively studied, with both experimental and computational results published in numerous technical reports and journals (Mitenkova et al., 1994; Hogenbirk et al., 1995; Brogli et al., 1989; Mathews and Chawla, 1990; Mathews, 1996). Currently, there is one pebble bed type reactor in operation, the HTR-10 in China (Zhong et al., 2001).

The unique features of pebble bed physics present both modeling challenges and simplifications. For the PBR, the cross section problem is compounded by the continuous mixing and reloading of fuel pebbles. The spectrum calculation is thus different than that of a LWR. One simplification is the ability to separate coolant and moderator effects. Because Helium is employed as the coolant, it is possible to ignore such impediments as phase changes and the void reactivity affects which complicate LWR analysis. Helium is also relatively transparent to neutrons, with the consequence that reactivity feedback effects from the coolant are non-existent.

There are, however, special considerations for PBR physics that demand a different approach to cross section generation than that employed by an LWR. Because

of the graphite moderation environment and low packing of the fuel grains (Stoker et al., 2002) there is a large scattering to absorption cross section ratio. Thus, the spectrum within a pebble is determined more by the burnup and leakage conditions in surrounding pebbles than within the considered pebble. This is in direct contrast to the spectrum of an LWR lattice, which is dominated by its own isotopics. In addition, the several layers of heterogeneity that characterize the PBR lattice can complicate the determination of the local resonance absorption at the grain and at the pebble levels (Kloosterman and Ougouag, 2005).

The core consists of a tall reactor vessel with spherical fuel elements that flow downward, accruing burnup along the trajectory. There are several variations upon this reactor type, with the two broadest being classified according to the pebble circulation policy: the Once Through Then Out (OTTO) cycle, and the recirculating core cycle. In addition, certain reactor designs call for flowing graphite reflector pebbles, of the same diameter as the fuel pebbles. The graphite pebbles, collectively known as the dynamic inner reflector, augment the reflective properties of the graphite bricks that line the core. This type of design is known as a two-flow zone PBR core.

For the recirculating core, a target burnup is defined which is usually higher than that of the LWR. When the fuel pebble drops out of the bottom of the core, it is examined to see if it has reached the target burnup. If the target is not met, it is reloaded at the top to traverse the core again, along with fresh fuel pebbles. The inner reflector pebbles are also reloaded to the top, but they contribute zero burnup.

The fuel elements themselves consist of heavy metal grains dispersed in a graphite matrix, which is further coated with a graphite shell, giving it the outer dimensions of a tennis ball.

Due to the nature of the continuous reloading scheme, there are several burnup states present in the core. Because of the large number and small size of fuel pebbles, it is difficult to affix a single burnup state to a specific reactor zone (Massimo, 1976; Gougar, 2004), and therefore the group constants are determined by the average composition of the zone. The use of an averaged spectral zone for spectrum calculations as a fuel cycle strategy was previously developed in the context of the DRAGON Project (Massimo, 1976) for high temperature graphite block reactors and in the V.S.O.P. code (Teuchert et al., 1980) for PBR's.

One of the chief difficulties in applying the LWR methodology to a PBR is that employing extensive tables of parameterized broad group cross sections can become difficult to implement in an equilibrium core analysis. With a lack of initial knowledge regarding the equilibrium solution, and also with the unknown convergence path to that solution, it would be necessary to resort to non-linear interpolation for the information between the cross section tabulations and to also employ a greater number of cross section data points. In order to address the uncertainty regarding the PBR extreme operating conditions, it would also be necessary to expand the operating envelope margins to accommodate the greater number of tabulations.

Traditionally among the older HTR fuel cycle codes, such as V.S.O.P. for the PBR (Teuchert et al., 1980) and BASS for the prismatic type (Massimo, 1976), , the time evolution of the core is explicitly tracked from the fresh core loading to the equilibrium

cycle, at which the reactor has reached a steady state. In these codes, it is customary to divide the core into spectral zones in which to perform the depletion calculations, a spectral zone being a collection of finite difference mesh points; the approach is to use the average composition of a spectral zone to calculate the group constants.

Because the depletion equations are one group, they can be very sensitive to spectral effects (Massimo, 1976). To calculate new group constants, spectrum calculations are performed in the broad spectral zones of the core. The time steps of the flux, burnup, and spectrum calculations are multiples of each other. In the BASS fuel cycle codes developed for the Dragon Project (Massimo, 1976), the spectrum calculations are performed with the forty three-group MUPO code. In the approach taken by the General Atomics burnup codes, a master twelve group cross section library is used throughout the calculation, with the cross sections being collapsed to one-group for depletion. To take into account the changes in the grain self-shieldings with fuel burnup, and in order to avoid frequent and expensive transport calculations at the grain level, fittings of the self-shielding as a function of the absorber concentration are pre-computed. This data is then used by the simulator during the calculation.

The PBR general fuel cycle analysis code V.S.O.P. is an established code that was developed in the Federal Republic of Germany to support the AVR Project (Teuchert et al., 1980; Schulten, 1989). It is an explicit time dependent code that actually tracks the physical development of the fuel cycle from fresh to equilibrium. In the simulation, batches of fuel are shuffled downward through the core, ejected from the bottom, and added back to the top. To update the spectrum during the fuel cycle, the THERMOS and

GAM-I modules are used (Finnan, 2004), coupled with a leakage feedback mechanism. An infinite medium, fresh library is employed to start the simulation.

In the fast energy range, the GAM-I calculation is completed in 68 energy groups from 10 MeV to 0.414 eV. The P1 approximation is applied to a homogenous distribution of materials. The neutron leakage into and out of spectral zones in V.S.O.P. is accounted for through buckling terms generated through the diffusion calculation. Resonance absorption is modeled by the use of user supplied self-shielding factors. In the epithermal region, bucklings are defined from the leakages in the following manner:

$$B_{S,h}^2 = \frac{L_{S,h}}{D_{S,h} \cdot \Phi_{S,h} \cdot V_S} \tag{2-1}$$

The symbol, "*S*" refers to the spectral zone, and "*h*" indicates the broad group. The numerator is the leakage, and the denominator consists of, respectively, the diffusion coefficient, the flux, and the zone volume.

The THERMOS calculation is completed for a one-dimensional cell in the thermal energy range, with 30 energy groups up to 2.05 eV. Self-shielding factors also need to be provided for this module. To account for neutron leakage at the lattice cell surface, an albedo is defined at the cell surface in terms of the spectral zone leakage, flux, volume, and the lattice cell volume and surface area.

In the older General Atomics codes that were applied to prismatic HTR's, it was found necessary to resort to zero-dimensional calculations in lieu of expensive three dimensional diffusion calculations for the flux (Massimo, 1976; van Howe, 1963). Thus, the zero-dimensional diffusion equation was reformulated such that the leakage per source neutron would be constant with burnup.

$$K_i = \frac{D_i \nabla^2 \phi_i}{\frac{1}{k_{eff}} \sum_j \nu_j \Sigma_{fj} \phi_j} \tag{2-2}$$

This source was incorporated to the source term of the zero-dimensional diffusion equation and significantly improved the calculation. This was done to take into account the leakages between zones and to avoid problems associated with the erroneous increase in the thermal incoming leakage from the reflector when the leakage, $D_i B_i^2 \phi_i$, is kept constant with burnup.

The equilibrium PBR fuel cycle code PEBBED under development at the INL (Gougar et al., 2002; Terry et al., 2002; Gougar, 2004) is unique in the sense that it is capable of converging to an asymptotic core solution directly by the use of a novel recirculation matrix, without the need for tracing explicit time steps. This presents an advancement over the older established PBR analysis code, V.S.O.P. An equilibrium solution is defined as a state in which the burnup, flux, power level, and the nuclide distribution do not change with time, and in reality it is achieved after a long time period of continuous refueling. With this analysis tool is the ability to predict an optimal fuel cycle with genetic algorithms, subject to a constrained variable (Gougar, 2004).

Since the energy spectrum corresponding to an asymptotic cycle is unknown initially, the current cross section methodology in use by PEBBED involves either interpolation from pre-computed libraries or iteration on several fuel cycle simulations. In the interpolation approach, burnup dependent cross section libraries are pre-computed for many depletion states. During the course of the simulation, the average burnup of a zone is 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. These are used to start a new PEBBED simulation to a new asymptotic solution, and the process is repeated until convergence.

The difficulty with the second approach is that there is no mechanism for updating the cross sections during the course of the solution, and this can be important since the macroscopic cross section is reconstructed for the flux solver, and the burnup calculation also depends upon the microscopic fission cross sections. In the first approach it may be difficult to fix a single burnup state to a set of zone averaged nuclide densities, as it is possible that the same burnup states in different parts of the reactor can exist with different nuclide distributions.

The chief assumption of the Spectral History Correction method developed in this work is that, due to the linearization of the decay chains, it is possible to track the isotopics strictly in terms of the U-235 density. Pre-computed cross section libraries are made as a function of this U-235 density, with the assumption that the macroscopic reaction dependent cross section may be built, with the corresponding, updated spectrum to be solved in that zone.

CHAPTER 3

THE METHOD

The PBR fuel cycle code PEBBED solves for the steady state, asymptotic solution directly without following a physically meaningful sequence of states. This asymptotic state is a true steady state in which the converged reactor variables such as the nuclide distribution, the flux, and the burnup distribution do not change with time. Generally, the older PBR codes (V.S.O.P. is the standard example) treat this time dependence explicitly, with the burnup calculation marching forward in time from the fresh state, depending upon the recirculation rule, and being directly coupled with the flux calculation.

Since PEBBED converges directly to a steady state equilibrium cycle using semi-analytical techniques, the entry plane burnup is another variable to be iterated upon, and its value in the cycle is determined by the recirculation rules for discharged pebbles. The general PEBBED algorithm is such that an initial zero burnup is assumed in the core, the flux solution is computed (in this case, with finite differences), the cell-wise burnup equation is calculated via the method of Terry et al. (2002) with an entry plane burnup of zero. Two nested burnup loops are then entered, with the outer burnup loop corresponding to the entry plane burnup (an unknown boundary condition governed by the recirculation policy), and the inner burnup loop that converges upon the cell-wise burnup and flux distribution. In PEBBED, the same grid is used for both the burnup and the flux such that the flat flux approximation for the burnup calculation is an accurate approximation.

However, with the new composition, due to depletion and to pebble movement, it is necessary to update the microscopic cross section library both for the depletion and the flux calculations. The microscopic library at infinite medium, mid-burnup conditions that was initially assumed is no longer accurate due to the composition change. The change in the cross sections due to both the composition change within a spectral zone and to composition change in a neighboring zone, is known as the spectral effect. The methodology to correct the cross section library as the core composition evolves is subsequently outlined.

3.1. The Core Calculation

The diffusion equation,

$$\nabla D_h^{(n,m)} \bullet \nabla \Psi_h^{(m)} + \Sigma_{t,h}^{(n,m)} \Psi_h^{(m)} = \sum_{h'=1}^{H} \Sigma_{s,h' \to h}^{(n,m)} \Psi_{h'}^{(m)} + \frac{1}{k} \chi_h \sum_{h'=1}^{H} \upsilon^{(n,m)}{}_{h'} \Sigma_{fh'}^{(n,m)} \Psi_{h'}^{(m)}, \qquad (3\text{-}1)$$

is solved for each finite difference cell. The indices "*n*", "*m*", and "*h*" stand for the spectral zone average composition state, the finite difference mesh, and the broad group number, respectively. PEBBED currently runs with six broad groups that are a variant of the V.S.O.P. boundaries (see Appendix A). In this methodology, a spectral zone is a collection of finite difference cells, and it represents an area of the reactor in which the spatial distribution of the microscopic cross section is assumed to be constant. On the same grid, PEBBED then uses the flux solution to compute the cell-wise burnup as a function of the change in fuel isotope nuclide densities, the flux, the cell volume, the fuel isotope fission cross sections, the energy per fission, and the initial mass of heavy metal in the cell. With the inner flux and burnup convergence, the entry plane burnup is

computed with the re-circulated nuclide densities, which are coupled to the discharged densities through a recirculation matrix.

When the composition in a finite difference cell depletes, the solutions to the depletion problem, the atomic densities, $N^{i,(n,m),}$, are then used to obtain the macroscopic cross sections for the next iteration step in the nodal diffusion equation solver, as:

$$\Sigma_{x,h}^{(n,m)} = \sum_i \sigma_{x,h}^{i,(n)} N^{i,(n,m)} \tag{3-2}$$

The symbol, "*x*", denotes the reaction type, and the symbol, "*i*" indicates the isotope. Note that the microscopic broad-group cross sections for each reaction type in the equation above are obtained by collapsing the fine-group cross sections given by the cross section generator for that particular composition state and therefore correspond to a specific fine-group flux spectrum.

$$\sigma_{x,h}^{i,(n)} = \frac{\sum_{g \in h} \sigma_{x,g}^{i,(n)} \Phi_g^{(n)}}{\sum_{g \in h} \Phi_g^{(n)}} \tag{3-3}$$

The index "*g*" in Eq. (3-3) indicates the fine group.

3.2. Spectral History Correction (SHC)

The chief correction in the methodology is the determination of the most correct microscopic cross section, $\sigma_{x,h}^{i,(n)}$ to reflect the average spectral zone composition and leakage with other zones. Initially, the fuel cycle simulation starts under the assumption that the cross section library may be generated at infinite medium, mid-burnup

conditions. However, this state does not correspond to what is obtained in the spectral zone as the fuel depletes. Thus, the spectrum used to produce the initial homogenized microscopic cross sections given by (3-3) is no longer accurate due to the isotopic changes within each node and to neutron leakage from other nodes. This implies that the homogenized microscopic cross sections have to be recalculated by performing a new cross-section calculation with the updated atom densities and a cross section generator or by table interpolation.

The philosophy behind Spectral History Correction is to recalculate the microscopic cross sections within a spectral zone for the effects of leakage and fuel burnup by using core information from the PEBBED simulation. To circumvent the use of the cross section generator and/or table interpolation, an approximation is made that the fine group, reaction type dependent macroscopic cross-section may be constructed with, in addition to the zone averaged nuclide densities, a set of pre-computed microscopic fine group libraries. These libraries are made from a recirculating pebble scheme of the PBMR-DIR design originating with PBMR Ltd. (Gougar, 2004), and extended to other PBR designs. This perturbation is expressed as,

$$\overline{\Sigma}_{x,g}^{(n+1)} \cong \sum_{i=1}^{I} \overline{\sigma}_{x,g}^{i,(n)} \overline{N}^{i,(n+1)} \,. \tag{3-4}$$

The symbol, "*I*" indicates the total number of nuclides. The bar over a quantity denotes that quantity averaged over a spectral zone. Note that the macroscopic cross section defined by Eq. (3-4) does not go directly into the diffusion equation defined by Eq. (3-1); instead it is used in the slowing down balance for an updated spectrum. The approximation in Eq. (3-4) is that the cross section libraries pre-computed at state (*n*) can

be used with the new nuclide densities to approximate the macroscopic cross section for the Spectral History Correction (SHC) at state (n + 1).

The pre-computed microscopic cross section libraries are completed for 141 fine groups with the cross section generator. The 141 fine groups are a subset of the General Atomics group structure for high temperature graphite reactors (see Appendix A). The nuclide densities used to construct the libraries are taken from an uncorrected PEBBED fuel cycle simulation. Equation (3-4) relies upon that phenomenon that, the finer the group width, the less the cross section depends upon the weighting spectrum shape.

The slowing down balance equation that is solved for the spectral zone spectrum is obtained from B_1 theory, with energy dependent bucklings (Massimo, 1976; Mathews, 1969).

$$D(E)\cdot B^2(E)\cdot\Phi(E)+\Sigma_t(E)\Phi(E)= \int_0^\infty \Sigma_s(E'\to E)\Phi(E')dE'+\frac{\chi(E)}{k_{eff}}\int_0^\infty \nu(E')\Sigma_f(E')\Phi(E')dE' \tag{3-5}$$

The buckling in Equation (3-5) approximates the spatial curvature of the flux and is classically defined in the following manner, where "Ψ" indicates the both the spatial and energy dependence of the flux.

$$B^2(E)=-\frac{\nabla^2\Psi(r,E)}{\Psi(r,E)} \tag{3-6}$$

In the standard multigroup treatment, the balance is integrated over an energy group g, such that groupwise reaction rates are conserved.

$$D_g B_g^2\Phi_g+\Sigma_{t,g}\Phi_g=\sum_{g'=1}^{G}\Sigma_{s,g'\to g}\Phi_{g'}+\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\Sigma_{f,g'}\Phi_{g'} \tag{3-7}$$

However, since the only leakage information from PEBBED has been averaged over the six broad groups, the six group buckling, averaged over *h* is employed in Eq. (3-7) as the leakage term.

With the construction of the fine group macroscopic cross-sections, the B_1 equation is discretized and solved for the homogenous fine group flux in each spectral zone.

$$\left(\overline{D}_g^{(n+1)} \overline{B}_{h,PEBBED}^{2,(n+1)} + \sum_{g' \neq g}^{G} \overline{\Sigma}_s^{(n+1),g \to g'} + \overline{\Sigma}_{n,\gamma}^{(n+1),g} + \overline{\Sigma}_f^{(n+1),g} - \overline{\Sigma}_{n,2n}^{(n+1),g} \right) \overline{\Phi}_g^{(n+1)} = \sum_{g' \neq g}^{G} \overline{\Sigma}_s^{(n+1),g' \to g} \overline{\Phi}_{g'}^{(n+1)} + \overline{\chi}_g^{(n)} \tag{3-8}$$

The eigenvalue is based on the spectrum iterate such that,

$$k_{eff} = \frac{\sum_{g=1}^{G} \overline{\nu} \cdot \overline{\Sigma}_f^{(n+1)} \overline{\Phi}_g^{(n+1)}}{\sum_{g=1}^{G} \left(\overline{\Sigma}_{n,\gamma}^{(n+1),g} + \overline{\Sigma}_f^{(n+1),g} - \overline{\Sigma}_{n,2n}^{(n+1),g} + \overline{D}_g^{(n+1)} \cdot \overline{B}_{h,PEBBED}^{2,(n+1)} \right) \cdot \overline{\Phi}_g^{(n+1)}} \tag{3-9}$$

Eq. (3-8) is calculated for G fine energy groups and I nuclides. The solution is completed recursively (Mathews, 1968). Convergence is achieved upon both the flux and the eigenvalue. The bar over the flux and cross sections denotes the spectral zone averaged quantities. The diffusion coefficient is defined from the transport coefficient in the standard manner.

$$\overline{D}_g^{(n+1)} = 1 \Big/ \left(3 \cdot \overline{\Sigma}_{tr}^{(n+1),g} \right) \tag{3-10}$$

The fission spectrum, $\overline{\chi}_g^{(n)}$, is stored with the reference precomputed cross-section libraries. The buckling is computed by PEBBED and averaged over the spectral zone under consideration as follows.

$$\overline{B}^2_{h,PEBBED} = \frac{\int \vec{J} \bullet d\vec{A}}{\int D \cdot \Psi dV} \tag{3-11}$$

MICROX-2 (Mathews, 1997) is the cross section generator code used to make the fine group libraries. It performs an extremely detailed pointwise resonance calculation with B_1 equations in the fuel and moderator regions, which in turn, are coupled by transfer probabilities. It also computes the ratio of the homogeneous to the heterogenous spectrums. This fine group ratio is stored with the libraries and used with Spectral History Correction.

This ratio, denoted a 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,

$$\mu_g^{(n)} = \frac{\overline{\Phi}^{(n)}_{g,homogeneous}}{\overline{\Phi}^{(n)}_{g,heterogeneous}}, \tag{3-12}$$

, the homogeneous flux solution from the solution of Eq. (3-8) may be corrected in the following manner.

$$\overline{\Phi}^{(n+1)}_{g,SHC} \cong \frac{\overline{\Phi}^{(n+1)}_{g}}{\mu_g^{(n)}} \tag{3-13}$$

In order to collapse the transport cross section, the current is approximated (Mathews, 1997) as,

$$\overline{J}^{(n+1)}_{g,SHC} \cong \overline{D}^{(n+1)}_{g} \left| \overline{B}_{h,PEBBED} \right| \overline{\Phi}^{(n+1)}_{g,SHC} \tag{3-14}$$

Finally, with the current and flux calculated, the fine group cross sections may be collapsed for the broad group cross sections for use in the PEBBED flux and depletion calculation. Again, the symbol "*x*" specifies all reactions excepting transport.

$$\overline{\sigma}_{x,h}^{i,(n+1)} \cong \frac{\sum_{g\in h}^{G} \overline{\sigma}_{x,g}^{i,(n)} \overline{\Phi}_{g,SHC}^{(n+1)}}{\sum_{g\in h}^{G} \overline{\Phi}_{g,SHC}^{(n+1)}} \tag{3-15}$$

The transport cross section is then collapsed with the current as,

$$\overline{\sigma}_{tr,h}^{i,(n+1)} \cong \frac{\sum_{g\in h}^{G} \overline{\sigma}_{tr,g}^{i,(n)} \cdot \left| \overline{J}_{g,SHC}^{(n+1)} \right|}{\sum_{g\in h}^{G} \left| \overline{J}_{g,SHC}^{(n+1)} \right|}. \tag{3-16}$$

3.3. The Fine Group Library

The chief assumption with SHC is that a fine group library that was pre-computed for representative PBR zone averaged densities can be used for the approximations in Eqs. (3-15), (3-16), (3-10), and (3-4). A PEBBED model was run to an equilibrium solution, with zone-averaged densities for the tracked nuclides used to make the libraries. Stored with the cross sections is the fine group fission spectrum for the mixture and the fine group modulation factor.

In reality, the decay chains that describe nuclide transmutation have several branches. However, PEBBED linearizes the decay chains such that, instead of the branches of a typical cycle, the one chain is reduced to two linear chains with a few common members (Gougar, 2004). It then becomes easier to track a zone-averaged mixture in terms of the density of U-235, the initial fissile nuclide. In addition to the relative depletion, the U-235 density would also indicate the amount of moderator pebbles in a spectral zone, with a lower density indicating more graphite pebbles. This

would correspond to the mixture area between the fuel pebbles of the core and the dynamic inner reflector.

With the pre-computed libraries in terms of the U-235 density, the SHC algorithm works by averaging the nuclides over a spectral zone. The amount of U-235 in the mixture is then matched to the closest relevant library for the state, (n).

The result is a methodology that calculates a new fine group spectrum within a spectral zone, taking into account the isotopics in that mixture through the nuclide densities, and the depletion level in neighboring spectral zones through the group dependent bucklings.

CHAPTER 4

RESULTS

To examine Spectral History Correction (SHC) as a viable method, several tests were formulated both inside and outside of PEBBED. Outside of PEBBED, the algorithm was coded such that it read the relevant libraries, constructed the cross section, and computed the spectrum and the current for that mixture. The terms of comparison were the eigenvalue, flux, and current errors. The implementation of SHC as a module within PEBBED was also completed and various test cases were analyzed and evaluated to demonstrate the robustness of SHC for different PBR designs and models. Broadly, then, Test I summarized the ability of SHC to calculate an accurate fine group spectrum. Test II dealt with the ability of SHC to compute cross sections for a recirculating PBR model design, PBMR-DIR. In Test III, PEBBED/SHC was applied to another variant of the PBMR-DIR design. The physical dimensions of the fuel pebbles, the PBR core, and figures of the spectral zones are given. For consistency, all calculations were completed at a core-averaged temperature of 1073 K.

4.1. Test I. Spectrum, Eigenvalue and Current Calculations

Two classes of problems were solved: the infinite medium problem and the finite medium problem. For the infinite medium problem, three cases are presented, in graduating level of severity for the method. For the finite medium problem, two cases are presented. Results from the spectra analysis are the eigenvalue errors, the root mean square percent errors for the current and flux, and the clock time. Both the method being

tested, SHC, and the benchmark (which varied per problem), MICROX-2, were computed for 141 fine groups. For the problems, three sets of densities and their corresponding libraries were used, as indicated in Table 4-1. The libraries for a particular state (*n*) contain the fine group microscopic cross-sections, the fine group fission spectra, and the modulation factors. The libraries in the SHC algorithm are tracked by U-235 density.

Table 4-1. Tracked Nuclide Densities in Different States [atoms/(barn-cm)].

	State (1)	State (2)	State (3)
He-4	1.87902E-04	1.87903E-04	1.87902E-04
C-nat	5.30624E-02	5.30624E-02	5.30624E-02
O-16	1.55509E-04	1.55509E-04	1.55509E-04
Si-nat	1.69997E-04	1.69997E-04	1.69997E-04
I-135	2.24068E-10	2.94455E-10	2.25584E-10
Xe-135	5.75486E-11	6.21882E-11	6.16492E-11
Pm-149	3.28192E-10	3.84220E-10	3.32420E-10
Sm-149	3.87275E-10	3.44817E-10	4.23445E-10
U-235	***2.91431E-06***	***3.16977E-06***	***3.41447E-06***
U-236	5.53713E-07	5.12100E-07	4.78237E-07
U-237	5.21064E-10	5.03090E-10	4.28973E-10
U-238	6.93187E-05	6.94833E-05	6.97322E-05
Np-237	1.97153E-08	1.79683E-08	1.35939E-08
Np-238	8.14609E-11	8.67524E-11	5.19943E-11
Np-239	1.43791E-08	1.64007E-08	1.38392E-08
Pu-238	4.70460E-09	4.10520E-09	2.51696E-09
Pu-239	3.75404E-07	3.63777E-07	3.74804E-07
Pu-240	1.95278E-07	1.81205E-07	1.75777E-07
Pu-241	1.25644E-07	1.13185E-07	1.00805E-07
Pu-242	5.95481E-08	5.20594E-08	3.42931E-08

For the infinite medium problems, three cases were analyzed. Taking the fine group libraries pre-computed at State (1), the macroscopic cross-sections were built (with Eq. (3-4)) at States (1), (2), and (3), named Case 1, Case 2, and Case 3. The fine group spectrum, current, and eigenvalue were calculated by Equations (3-8) through (3-14). These cases are indicated in Table 4-2.

For the finite medium cases, 6 group bucklings taken from a PEBBED solution were used in both the MICROX-2 and SHC models. In Case 4, fine group, infinite medium libraries at State (1) were combined with nuclide densities at State (2) and the 6 group bucklings to yield a spectrum, eigenvalue, and current. Each broad group buckling corresponded to a fine group buckling for the fine group calculation. Case 5 was similar, but it stretched SHC from State (1) to State (3). Case 5 was the most severe case for SHC. Both Cases 4 and 5 combined an infinite medium library with a finite medium calculation. These cases are also indicated in Table 4-2.

Table 4-2. Case Descriptions.

	Fine Group Library (*n*)	**Nuclide Densities (*n*+1)**	**SHC Calculation**	**MICROX-2 Calculation**
Case 1	State (1)	State (1)	Infinite	State (1); Infinite
Case 2	State (1)	State (2)	Infinite	State (2); Infinite
Case 3	State (1)	State (3)	Infinite	State (3); Infinite
Case 4	State (1)	State (2)	Finite	State (2); Finite
Case 5	State (1)	State (3)	Finite	State (3); Finite

All five cases were completed and the terms of comparison are indicated in Table 4-3. The reference problem for each case was a fine group (141 groups) MICROX-2 calculation corresponding to that state. The % Root Mean Square (RMS) of the error for the current and the flux was calculated according to Eqs. (4-1) and (4-2).

Table 4-3. SHC vs. MICROX-2 at 141 Groups

	Case 1	Case 2	Case 3	Case 4	Case 5
Eigenvalue Error (mk)	0.00	-0.14	0.18	-0.10	-0.41
Flux % RMS	1.971140E-05	1.723770E-02	3.088220E-02	1.638950E-02	2.960720E-02
Current % RMS	2.529720E-04	1.735220E-02	3.132650E-02	1.330050E+00	1.330410E+00
Eigenvalue Iterations	118	82	104	184	188
SHC Clock Time [s]	1.73400	1.75000	1.79700	1.84300	1.81300
MICROX Clock Time [s]	3.6875	3.7188	3.6406	3.9375	4.3438
Bucklings (Groups 1 to 6)	3.19155E-04, 2.92348E-04, 2.67861E-04, 2.88940E-04 2.49959E-04, -6.01170E-05				

$$\%\ RMS = 1/(G-1)\cdot\sqrt{\sum_{g=1}^{G} e_g^2} \tag{4-1}$$

$$e_g^{\phi} = 100*\left(\varphi_g^{SHC} - \varphi_g^{MICROX}\right)/\varphi_g^{MICROX}$$
$$e_g^{J} = 100*\left(J_g^{SHC} - J_g^{MICROX}\right)/J_g^{MICROX} \tag{4-2 (a)(b)}$$

Since Case 1 matched libraries and densities at the same state, it yielded the lowest errors. As can be expected given the larger perturbation for Case 5 (Case 5 was based on an infinite medium library,) it yielded a larger error for the current. However, as these differences are for the fine multigroup calculation, and also since the current is only used to collapse the transport cross section, the collapsed broad group cross sections are more of interest.

To this end, collapsed broad group microscopic cross sections were selected for comparison based on their magnitude. A realistic case that could arise during a PEBBED/SHC simulation, Case 4, was evaluated. A cross section comparison was also given for Case 1. Collapsed SHC microscopic cross sections for Case 4 were compared to the true 6 group MICROX-2 cross sections at that leakage and isotopic state. These were Group 6 Graphite Scatter, Group 6 Sm-149 Transport, Group 4 U-238 Capture, and Group 6 U-235 Fission. These are indicated in Table 4-4.

Table 4-4. Collapsed 6 Group Cross Section Comparison.

Case 1	**SHC**	**MICROX**	**Relative % Error**
G6 Graphite Scatter	7.25865E+00	7.25865E+00	0.00000E+00
G6 Sm-149 Transport	3.32306E+04	3.32307E+04	-3.00927E-04
G4 U-238 Capture	3.81130E+01	3.81130E+01	0.00000E+00
G6 U-235 Fission	2.28571E+02	2.28571E+02	0.00000E+00
Case 4	**SHC**	**MICROX**	**Relative % Error**
G6 Graphite Scatter	7.24823E+00	7.24874E+00	-7.03571E-03
G6 Sm-149 Transport	3.32999E+04	3.36589E+04	-1.06658E+00
G4 U-238 Capture	3.81789E+01	3.81462E+01	8.57228E-02
G6 U-235 Fission	2.28874E+02	2.28814E+02	2.62222E-02

4.2. Test II. PEBBED/SHC: Fuel Cycle Calculations for the PBMR-DIR

The SHC algorithm was coded and fully implemented into PEBBED as a subroutine and called with leakage and burnup updates and broad group cross section arrays. The subroutine was inserted at two points in PEBBED. The first subroutine call occurred during the initial flux solution for the fresh core loading. The next subroutine call occurred within the module that controls the asymptotic solution, within the outer burnup loop. As per Terry et al. (2002) and Gougar (2004), in the outer burnup loop, the code converges on an entry plane burnup profile; this depends on the recirculation scheme of discharged pebbles. The inner burnup loop converges upon the flux and burnup distribution within the core. The PEBBED/SHC method was analyzed in terms of the core equilibrium eigenvalue, the fission density, the power peaking factor, and the relative flux error.

The benchmark problem for comparison was chosen to be the case in which PEBBED calls a subroutine which writes an input deck and calls the cross section generator through a system call, with updates of either the bucklings or the depletions, or a combination of both, depending upon the parameter studied. Thus, during the convergence to an equilibrium fuel cycle, MICROX-2 was called repeatedly to update the microscopic cross sections for the flux and burnup calculations. MICROX-2 was run for the six broad groups in use by PEBBED. It was necessary to recompile MICROX-2 to accommodate the increased iterations necessary for some of the leakage patterns encountered with the cross section updates. This is detailed in Appendix A.

The initial PBR reactor design chosen for testing was a variation of the PBMR-DIR theme initially designed by PBMR Ltd. of South Africa. The considered design for this study was later adapted and improved at the INL for use with PEBBED pebble bed reactor design optimization studies (Gougar, 2004). The 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 downwards 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 economics, the fuel pebbles are burned to a very high burnup (80 MWD/kg-U) and consequently discharged. In this design, 75 % of the core total pebble flow is in the outer fuel zone annulus.

The specific PEBBED model incorporated five flow channels for the entire 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 partition for each channel is approximately ~0.20. The second channel includes both graphite and fuel pebbles. In the PBR design considered for this study, the fuel pebble 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, as already outlined, 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 in nature, encompassing a cylindrical core with 30 radial cells, 88 axial cells, and 1 cell in the azimuth 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. More dimensions of the

PBMR-DIR are outlined in Table 4-5, and a two-dimensional slice of the core with the spectral zone map is illustrated with Figure 4-1. Table 4-6 gives the key for Figure 4-1.

Table 4-5. 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

The microscopic cross sections which were tracked by PEBBED and which were recalculated by SHC included the scattering matrix, the transport cross sections, the absorption cross sections, nu-fission, and the fission cross sections. These cross sections were calculated for all nuclides present in Table 4-1.

In addition, in this PEBBED model the cell nuclide densities are homogenized over a Body Centered Cubic (BCC) lattice arrangement. The core is initially loaded with fresh fuel pebbles and graphite pebbles. Spectral zones 5 and 6 correspond to fuel pebbles. Spectral zone 2 is the graphite pebble region, and spectral zones 3 and 4 define the graphite-fuel mixture region. PEBBED runs with six broad groups, whose upper energies are listed in Appendix A.

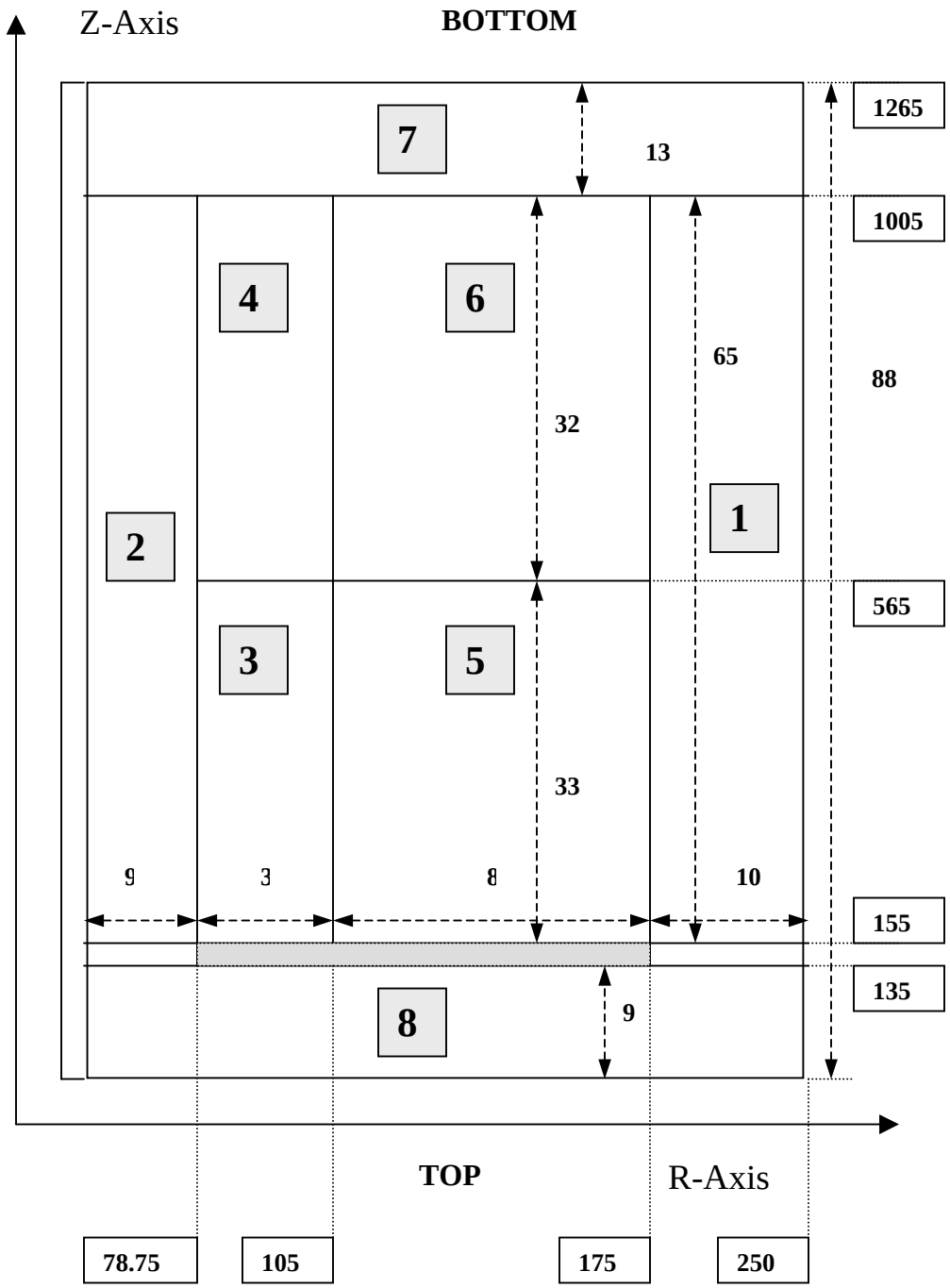

Figure 4-1. PBMR-DIR Schematic.

Table 4-6. Key for Figure 4-1.

Spectral Zone	Description
1	Side graphite reflector.
7	Bottom graphite reflector.
8	Top graphite reflector.
2	Dynamic flowing graphite pebbles.
3 4	Mixing zone, graphite and fuel pebbles.
5 6	Fuel zone, fuel pebbles.
Symbol	**Description**
#	Indicates finite difference cells.
#	Indicates length dimension in [cm].

The 141 fine group cross section libraries on which the SHC subroutine is based were generated using the NJOY/MICROR/MICROX-2 system (MacFarlane and Muir, 1999; Pelloni, 1992). These libraries were constructed by running an uncorrected PBMR-DIR fuel cycle calculation, with collected nuclide densities being used to write MICROX-2 input decks and to create the libraries. The 6-group library necessary to start the PEBBED simulation was also generated with the same cross section system at the same burnup.

In the MICROX-2 model, it is necessary to homogenize the outer graphite layer with the Helium and to correct for lattice effects through the use of a pebble-to-pebble Dancoff factor, which was calculated analytically (Bende et al., 1999). The dimensions of the BCC lattice, which formed the basis of the SHC methodology and PEBBED models, along with a representative pebble Dancoff factor are given in Table 4-7. For the benchmark problem, the Dancoff factor was recalculated from the coded analytic formulae at each cross section update. This was to ensure consistency between the Dancoff and the actual outer layer graphite density obtained in the moderator region.

Table 4-7. Pebble Dimensions and Typical Dancoff Factor: 61 % BCC.

Outer radius of BCC pebble lattice [cm]	3.53735
Lattice pitch [cm]	7.18430
Moderator region total cross section [cm^{-1}]	0.166941
Pebble lattice Dancoff factor	0.446051
Pebble packing fraction	0.61

To quantify the relative effects of both the leakage and the depletion, two tests were formulated and setup as models with the existing methodology: an infinite medium problem, and a finite medium problem.

4.2.1. Test II.A. The Spectral Effect

The first test, II.A, was formulated to quantify the extent of the change in the fuel burnup of the isotopic cross sections upon the end of fuel cycle converged core parameters. The re-computation of the cross sections for only depletion effects was accomplished through the solution of the infinite medium slowing down balance (Eq. (3-8) with B_h^2 = 1.00e-10), within each spectral zone of the fuel core. That is, the net leakage effect upon the spectrum within the spectral zone was not considered; the spectral effect within the considered zone was isolated.

The case in which a PEBBED simulation was run to a converged fuel cycle without cross section update is denoted the Uncorrected Case (UC). In this case, the same microscopic cross section library is used throughout the calculation. The UC library is constructed for an infinite medium at a burnup of ~ 45 MWD/kg.

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 for this benchmark.

The results for the infinite medium SHC and the infinite medium benchmark problem are indicated in Table 4-8.

Table 4-8. SHC vs. Benchmark for Fuel Burnup Only (PBMR-DIR).

	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

The use of the infinite medium SHC algorithm with PEBBED led to considerable improvement in predicting the core equilibrium eigenvalue. The converged PEBBED values were taken from PEBBED output files. 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 about ~2.9 mk. This is almost a ~ 9 X improvement in the neutron balance of the converged core. The relative error for the SHC for the maximum power peaking factor (PPF) and mean power peaking factors was 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.

Regarding the flux and fission density, the % Root Mean Square (RMS) error was computed. 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 (spectral zones 2 through 6). For the fission density, the % RMS was also

computed for the core cells. The fission density improvement was nearly ~ 24 X, and the one group flux improvement was almost ~ 10 X.

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, representing a savings of almost 2 X.

4.2.2. Test II.B. Leakage and Spectral Effects

The second test case, II.B, was completed to demonstrate the sensitivity of the converged core parameters on both the spectral zone isotopics and the net neutron leakage from neighboring spectral zones. The re-computation of the spectrum was accomplished through the solution of the B1 slowing down balance, within each spectral zone of the fuel core. The benchmark problem took zone averaged nuclide densities and net leakages as arguments from the PEBBED simulation. The results for PEBBED/SHC and the finite medium benchmark problem are given in Table 4-9.

Table 4-9. SHC vs. Benchmark with Burnup & Leakage Effects (PBMR-DIR)

	Local cross sections from MICROX (Benchmark)	Global cross sections only (UC)	Error	SHC-generated local cross sections	Error
Eigenvalue	*1.0375539*	*1.0409036*	*3.350*	*1.0368915*	*-0.6624*
Max. PPF	*1.68*	*1.65*	*-1.79*	*1.68*	*0*
Mean PPF	*1.56*	*1.53*	*-1.92*	*1.56*	*0*
	SHC % RMS Error			**UC Relative % RMS Error**	
Flux	*6.72E-03*			*3.08E-02*	
Fission Density	*9.61E-03*			*1.18E-01*	

As in the infinite medium problem, the PEBBED/SHC combination gave a great improvement in core equilibrium eigenvalue, power peaking factor, flux, and fission density. PEBBED/SHC under predicted the core eigenvalue by ~ -0.66 mk, as compared to the benchmark. The uncorrected case (UC) over predicted the core equilibrium eigenvalue by about ~3.4 mk. This is approximately a ~ 5 X improvement in the core eigenvalue. The relative error for the SHC for the maximum power peaking factor (PPF) and mean power peaking factors was 0.0 %, which is excellent, as opposed to the uncorrected case (UC) errors of ~-2.4 and ~-2.6 %. The fission density improvement was almost ~ 12 X, and the flux improvement was nearly ~ 5 X.

Another set of experiments was completed to quantify which spectral zone update would have the most impact on converged core parameters. To this end, several PEBBED runs were completed in which the cross sections from only one spectral zone were updated during the simulation. The results and their errors to the benchmark (in which MICROX was called only at that spectral zone), in terms of the power peaking factors (PPF) and eigenvalue, are given in Table 4-10. The differences between the SHC results and the UC cases are also indicated.

In terms of the core eigenvalue, recalculating the cross sections in Spectral Zone 2 has the most impact. The difference in [mk] between the SHC and UC cases is about ~ - 2.4. However, when considering the maximum power peaking factor of the core, updates in Spectral Zones 3 and 4 had the most impact. This is to be expected since the single broad group library employed in the UC case is extremely inaccurate for those zones containing graphite pebbles (it considers only fuel pebbles), and recalculating the cross sections with instantaneous core information would make a large difference.

Table 4-10. Cross Section Update per Spectral Zone.

	Zone #2	Zone #3	Zone #4	Zone #5	Zone #6
Max PPF	*1.64*	*1.71*	*1.71*	*1.65*	*1.65*
Mean PPF	*1.51*	*1.55*	*1.56*	*1.52*	*1.52*
Eigenvalue	*1.0384681*	*1.0397557*	*1.040729*	*1.0394164*	*1.0404001*
Error	**SHC vs. Benchmark (Zone Update)**				
Max PPF (% Relative)	*0.00*	*0.00*	*0.00*	*-0.60*	*0.00*
Mean PPF (% Relative)	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*
Eigenvalue (mk)	*-0.0646*	*0.006*	*-0.0053*	*-0.2891*	*-0.3005*
Differences	**SHC (Zone Update) vs. UC**				
Max PPF (% Relative)	*-0.61*	*3.64*	*3.64*	*0.00*	*0.00*
Mean PPF (% Relative)	*-1.31*	*1.31*	*1.96*	*-0.65*	*-0.65*
Eigenvalue (mk)	*-2.4355*	*-1.1479*	*-0.1746*	*-1.4872*	*-0.5035*

4.3. Test III. PEBBED/SHC: Calculations for a Modified PBR Design

Since the fine group libraries used in SHC were constructed with the previously described PBMR-DIR reactor type, a modification of the PBMR-DIR design (MPBR) was performed to ascertain the appropriateness of SHC for other PBR designs.

There were several differences between the two designs. The Modified PBR had pebble flow rate of 3000 pebbles per day (as opposed to 5140 pebbles/day). There was no dynamic inner reflector, i.e. the core contained only fuel pebbles, and the ex-core decay time for the fuel pebbles was 40 hours. The last difference pertained to the manner in which the fuel pebbles were recirculated. The circulation mode was random recycle, meaning that the discharged pebbles were randomly assigned to one of the five flow channels at the top of the core.

The results are presented in Table 4-11.

Table 4-11. SHC vs. Benchmark with Burnup & Leakage Effects (MPBR).

	Local cross sections from MICROX (Benchmark)	**Global cross sections only (UC)**	**Error**	**SHC-generated local cross sections**	**Error**
Eigenvalue	*1.0425736*	*1.0491198*	*6.546*	*1.0419612*	*-0.6124*
Max. PPF	*1.29*	*1.3*	*0.78*	*1.29*	*0*
Mean PPF	*1.12*	*1.14*	*1.79*	*1.12*	*0*
	SHC % RMS Error			**UC Relative % RMS Error**	
Flux	*5.58E-03*			*1.30E-01*	
Fission Density	*7.38E-03*			*1.25E-01*	

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

5.1. Discussion

A method is derived, implemented, and presented which addresses a chief concern in PBR equilibrium core analysis: the generation of physically accurate neutron-nuclear cross sections. The method, Spectral History Correction (SHC), tackles this problem by approximating a fine group spectrum for those regions of the core, named spectral zones, in which the cross sections are assumed as constant. This is accomplished by approximating the fine group spectrum by the solution of the slowing down balance equation. The method depends upon the pre-computation of fine group cross-section libraries, fission spectra, and modulation factors, which are tracked by the density of Uranium 235. The libraries are combined with nuclide densities from the spectral zone to construct reaction dependent macroscopic cross sections for the balance equation. The result is a method that is a compromise between data storage and between computations; SHC presents an alternative to the more traditional approach of interpolation and parameterization. In addition, SHC is simple to implement within the PBR simulator code.

The method is tested both inside and outside of the PBR simulator. Outside the PBR simulator, SHC was demonstrated to reproduce the fine group spectrum accurately

for both an infinite medium and a finite medium, despite the severe approximation of an infinite medium fine group library. It also gives an approximation for the current that is workable within the constraints. The ability of the method to collapse microscopic cross sections is demonstrated for selected isotopes and groups.

When implemented in the PBR fuel cycle code, PEBBED, the method gives very encouraging results when compared to the benchmark problem. Progress is measured in terms of the converged core eigenvalue, power peaking factor, flux, and fission density. Three cases are considered: the infinite medium problem for a PBMR-DIR, the finite medium problem for the same reactor, and the finite medium problem for a modified PBR design. Since the fine group libraries are constructed from a PBMR-DIR simulation, the success of SHC in another PBR design with different circulation patterns is very encouraging.

The conclusion is that SHC is a cross section methodology that is relatively simple to implement and computationally inexpensive within the context of PBR equilibrium calculations.

5.2. Future Work

There are several immediate goals for the method that, with their full success, would demonstrate whether the method could be viable when applied to a diversity of reactor problems.

The most pressing goal is the full testing of this method against a wider variety of PBR designs and considerations. The main advantage of SHC is its speed when compared against the more detailed resonance/transport spectrum calculation, and it is

expected that this will become more apparent when a greater number of spectral zones are employed in the reactor and when optimization problems are considered.

The second goal would be the implementation of a Doppler broadening capability such that the temperature gradients within the reactor core are captured. Already, the libraries are generated at the core averaged hot temperature condition, and thus the average temperature is captured. However, it is known that local temperature gradients, between different parts of the reactor do affect the local resonance absorption and the moderating power of graphite, significantly altering the local neutron balance.

APPENDIX A

SUPPLEMENT

Table A-1. 141 Fine Group Energy Structure.

1.49182E+07	1.34986E+07	1.22140E+07	1.10517E+07	1.00000E+07	9.04837E+06
8.18731E+06	7.40818E+06	6.70320E+06	6.06531E+06	5.48812E+06	4.96585E+06
4.49329E+06	4.06570E+06	3.67879E+06	3.32871E+06	3.01194E+06	2.72532E+06
2.46597E+06	2.23130E+06	2.01897E+06	1.82684E+06	1.65299E+06	1.49569E+06
1.35335E+06	1.22456E+06	1.10803E+06	1.00259E+06	9.07180E+05	8.20850E+05
7.42736E+05	6.72055E+05	6.08101E+05	5.50232E+05	4.97871E+05	4.50492E+05
4.07622E+05	3.68832E+05	3.33733E+05	3.01974E+05	2.73237E+05	2.47235E+05
2.23708E+05	2.02419E+05	1.83156E+05	1.65727E+05	1.49956E+05	1.35686E+05
1.22773E+05	1.11090E+05	8.65170E+04	6.73795E+04	5.24752E+04	4.08677E+04
3.18278E+04	2.47875E+04	1.93045E+04	1.50344E+04	1.17088E+04	9.11882E+03
7.10174E+03	5.53084E+03	4.30743E+03	3.35463E+03	2.61259E+03	2.03468E+03
1.58461E+03	1.23410E+03	9.61117E+02	7.48518E+02	5.82947E+02	4.53999E+02
3.53575E+02	2.75364E+02	2.14454E+02	1.67017E+02	1.30073E+02	1.01301E+02
7.88932E+01	6.14421E+01	4.78512E+01	3.72665E+01	2.90232E+01	2.26033E+01
1.76035E+01	1.37096E+01	1.06770E+01	8.31529E+00	6.47595E+00	5.04348E+00
3.92786E+00	3.05902E+00	2.38237E+00	2.19750E+00	1.91500E+00	1.85000E+00
1.69500E+00	1.43250E+00	1.30000E+00	1.25000E+00	1.13375E+00	1.12250E+00
1.08000E+00	1.06000E+00	1.04625E+00	9.90000E-01	9.80000E-01	9.30000E-01
8.91500E-01	8.73000E-01	7.50000E-01	6.79000E-01	6.25000E-01	5.88750E-01
5.72500E-01	5.05500E-01	4.81250E-01	4.75000E-01	4.60000E-01	4.21000E-01
4.07000E-01	3.50000E-01	3.30000E-01	3.10000E-01	2.90000E-01	2.70000E-01
2.50000E-01	2.30000E-01	2.17500E-01	1.80000E-01	1.20000E-01	9.50000E-02
8.50000E-02	7.50000E-02	6.50000E-02	5.87500E-02	3.13250E-02	2.51500E-02
1.07500E-02	6.75000E-03	3.75000E-03	0.00000E+00		

Table A-2. 6 Broad Group Energy Structure.

	Group 6	Group 5	Group 4	Group 3	Group 2	Group 1	
E_6	E_5	E_4	E_3	E_2	E_1	E_0	
0.0	1.86	2.38	29.0	7102	0.111E6	1.49E7	

Table A-3. Recompiling of MICROX-2 for the Finite Medium Benchmark.

Original	NLOOP.LT.10 on line # SPECT.899
Change	NLOOP.LT.500 on line # SPECT.899

Table A-4. Fresh Fuel Homogenized Densities.

Composition Region	BCC Homogenized Atom Density (atoms/barn-cm)
Fuel Pebble Isotopes	
Natural Carbon	5.264E-02
U-235	9.949E-06
U-238	1.126E-04
O-16	2.458E-04
Natural Silicon	2.687E-04
He-4	1.830E-04
Reflector Isotopes	
Natural Carbon	7.671E-02
Gas Plenum Isotopes	
He-4	5.076E-04
Graphite Pebble Isotopes	
Natural Carbon	5.379E-02
He-4	1.964E-4

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