ON THE EVALUATION OF PEBBLE BEAD REACTOR CRITICAL EXPERIMENTS USING THE PEBBED CODE

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Abstract – Critical experiments pose a particular but necessary challenge to validating pebble bed reactor design codes. Fuel and core heterogeneities, impurities in graphite, variable packing of pebbles, and moderately strong neutronic coupling are among the factors that inject uncertainty into the results obtained with lower fidelity core physics models. Some of these are addressed in this study. The PEBBED pebble bed reactor fuel management code under development at the Idaho National Laboratory is designed for rapid design and analysis of pebble bed high temperature reactors (PBRs). Embedded within the code are the THERMIX-KONVEK thermal fluid solver and the COMBINE-7 spectrum generation code for inline cross section homogenization. Because 1D symmetry can be found at each stage of core heterogeneity: spherical at TRISO and pebble levels, and cylindrical at the control rod and core levels, the 1-D transport capability of ANISN is assumed to be sufficient in most cases for generating flux solutions for cross section homogenization. Furthermore, it is fast enough to be executed during the analysis or the equilibrium core.

Multi-group diffusion-based design codes such as PEBBED and VSOP are not expected to yield the accuracy and resolution of continuous energy Monte Carlo codes for evaluation of critical experiments. Nonetheless, if the preparation of multigroup cross sections can adequately capture the physics of the mixing of PBR fuel elements and leakage from the core, reasonable results may be obtained.

In this paper, results of the application of PEBBED to two critical experiments (HTR Proteus and HTR-10) and associated computational models are presented. The embedded 1-D transport solver is shown to capture the double heterogeneity of the pebble fuel in unit cell calculations. Eigenvalue calculations of a whole core are more challenging, particularly if the boron concentration is uncertain. The sensitivity of major safety parameters to variations in modeling assumptions, however, is shown to be minimal.

The embedded transport solver can also be used to obtain control rod worths but only if the local spectrum is adequately captured in the control rod region. Results are compared to those of other codes as well as Core 4 of the HTR-Proteus experiment which contains partially inserted rods. They indicate the need for a reference solution to adjust the radius of the graphite in the control rod unit cell or some other method for obtaining the correct spectrum in these regions.
I. INTRODUCTION

Development of the PEBBED code [1] commenced in 1999 as part of a new research and development effort at the Idaho National Laboratory to investigate the technical viability of the modular pebble bed high temperature gas-cooled reactor. The code was meant to perform rapid sensitivity and design studies of pebble bed reactors (PBR) featuring online fuel loading and recirculation in support of fuel and material qualification and general plant studies. From the beginning, it was designed to skip the ‘running-in’, or pre-equilibrium period of PBR operation and converge quickly and directly upon the equilibrium core. Although an earlier version of the VSOP [2] code was available, a new ‘homegrown’ analysis capability was considered more suited to project needs and would be amenable to modification and development using modern programming techniques. Indeed, the capabilities of the code have grown in response to requests to perform a wide variety of analysis in support of code-to-code comparisons, accident analyses, fuel performance, small modular reactor design, alternative fuel cycles, and nonproliferation studies.

Validation of equilibrium PBR core models, PEBBED or any other code, is not yet possible as no pebble bed reactor has attained an equilibrium burnup profile. The HTR-PM, under construction in China and scheduled for critical operation in 2016[3], may provide suitable data within a few years of full power operation. Until such data becomes available, only individual components of multiphysics codes such as PEBBED can be validated by isolating the appropriate solvers and applying them to simpler, non-integrated models of experiments. The neutron transport solver can be validated to some extent against zero-burnup critical experiments, the thermal-hydraulic solver against heated test facilities, and the depletion solver against available burnup data. These are complemented by numerous code-to-code comparisons (loosely labeled as ‘benchmarks’). The accumulated results of these calculations may be sufficient to obtain a license for construction and start-up testing of a power plant but long-term operation must be accompanied by a series of measurements of rod worth, feedback, coefficients, flux and temperature data and, eventually, burnup analysis of discharged pebbles.

In this study, results from two critical experiments were used to assess the neutron spectrum and diffusion solvers in PEBBED. The effect on the core eigenvalue of different leakage approximations and pebble packing assumptions were computed. Control rods pose a particular modeling challenge as they are placed in the side reflector and thus cannot be embedded in an ‘assembly’ transport model.

This is not meant to be a full-scale sensitivity analysis of the type performed in proper reactor experiment benchmarking efforts. Such projects exploit high resolution, high fidelity modeling techniques which are not generally necessary for design studies. It does, however, yield an indication of the variability of full core neutronic results as obtained from low order PBR fuel management codes and the sensitivity of certain safety significant parameters to those variations.

II. MULTISCALE CORE MODELING WITH PEBBED

II.A. Overall Capabilities and Comparisons

PEBBED iterates between diffusion, burnup, thermal-fluid, and spectrum solvers to converge directly upon the equilibrium core profile. The code can account for variable packing density and velocity of pebbles, overlap of up to 3 resonances, different pebble types, and arbitrary loading and recirculation patterns. A unique treatment of pebble flow allows complex flow patterns to be modeled using a few pre-computed parameters, enabling efficient optimization of core geometry and loading patterns. A full description of its capabilities is given in [4]. As with most types of reactors, however, the key to accurate neutronic analysis is in capturing the local spectrum for generating few group cross sections.

II.B. Multiscale Cross Section Preparation

As with VSOP, a PEBBED model of a PBR core is divided somewhat arbitrarily into ‘spectral zones’ consisting of batches of pebbles or sections of the reflector. The composition within the zone is assumed to be a homogeneous mixture of the different pebbles or reflector structures within the zone. A slowing-down/resonance calculation is performed on the homogeneous fuel mixture with corrections for the heterogeneity of the fuel (for example, using collision probabilities and Dancoff factors to adjust the cross sections for the probability of a neutron leaving a fuel particle having its first
collision in another). The infinite medium spectrum is then adjusted using some approximation of the inter-zone leakage before it is used to generate few group cross sections for the core-wide diffusion model. This correction is important in PBRs as the mean free path of neutrons is large relative to the size of the spectral zone and inter-zone coupling can be significant.

In VSOP, inter-zone leakage is captured as a DB₂ correction to the macroscopic absorption cross section in the slowing down equation in which D refers to the diffusion coefficient and B₂ is the buckling obtained from the inter-zone leakage computed in the four-group core diffusion solution. PEBBED takes this approach a step further with a multi-scaled application of a discrete ordinates transport code [5]. Explicit one-dimensional (spherical) models of fuel particles are used to homogenize those structures and feed the resulting data to another transport model of a pebble (fuel region, outer graphite shell, and surrounding coolant). The spectrum generated by this model can be corrected for leakage (a la VSOP) to generate few group pebble cross sections. Instead, however, PEBBED performs one more transport calculation of a cylindrical wedge of the core and radial reflector using those cross sections. The inter-zone radial leakage is thus obtained from the transport solution in 167 energy groups. Axial leakage (and azimuthal in 3D models) is captured in few-group DB₂ terms as in VSOP. Given that most PBR cores designed over the past 30 years have large aspect ratios (height/diameter), leakage is usually greatest in the radial direction so this approach theoretically captures the leakage spectra with greater fidelity than the simple leakage model assumed for VSOP. The aspect ratios for critical experiments are usually much lower so the improvement may not be as significant in these cases (see Table 1).

### Reactor | Aspect Ratio | Fast | Thermal
---|---|---|---
Proteus | 1.2 | 2.6 | 8.5
HTR-10 | 0.68 | 1.3 | -2.7* 
PBMR-400 | 3.0 | 52 | 2.2

*negative value indicates that the net radial leakage is negative (into the core) while net axial leakage is positive

Table 1: Ratio of Radial to Axial Leakage in Reactors Modeled in this Study

The 1-D transport models run sufficiently fast to allow inline cross section updating. Furthermore, this multi-stage transport calculation enables explicit modeling of absorber elements (rods or absorber spheres, aka KLAK) located in the reflector using the current from the core as the neutron source for homogenization.

This is all well and good in theory but full validation of the approach remains to be completed. Progress toward that end was made in this study.

### III. NUMERICAL CONFIRMATION

Though not validation per se, comparison of the results of unit cell models of pebbles helps to identify modeling errors and to identify sources of uncertainty in the cross section generation process. Such a set of computational exercises was specified as part of the HTR Proteus series of critical experiments conducted using the Proteus facility at the Paul Scherrer Institute in Switzerland in the early 1990s.

Proteus was a zero-power research reactor with a cylindrical graphite annulus surrounding a central cylindrical cavity. The graphite annulus remained basically the same for all experimental programs, but the contents of the central cavity are changed according to the type of reactor being investigated. Through most of its service history, PROTEUS has represented light-water reactors, but from 1992 to 1996 PROTEUS was configured as a pebble-bed reactor (PBR) critical facility and designated as HTR-PROTEUS. During this period, thirteen critical configurations were assembled and various reactor physics experiments were conducted [6]. These experiments provided data for a number of reactor physics benchmark evaluations and associated computational exercises, some of which were exploited in this study and are described in the next sections.

#### III.A. Unit Cell Calculation

Calculational benchmark problems based on some of the initially proposed configurations for the critical experiments in the PROTEUS facility were prepared and distributed by PSI to the organizations in the CRP in 1990 [7]. The benchmarks consist of six graphite reflected 16.76% enriched-uranium pebble-bed systems of three different lattice geometries and two different moderator-to-fuel pebble ratios (2:1 and 1:2).

For the unit cells the following parameters were requested (among others):

- \( k_e \): no leakage from the cell
- \( B^2 \): critical buckling
- \( k_{B2} \): production rate/absorption rate in the critical cell
- \( M^2 \): migration area and the following spectral indices,

\[
\rho_{28} = \text{ratio of epithermal-to-thermal U-238 captures}
\]
$\delta_{25}$ = ratio of epithermal-to-thermal U-235 fissions
$\delta_{28}$ = ratio of fissions in U-238 to fissions in U-235
$C^*$ = ratio of captures in U-238 to fissions in U-235

Double-heterogeneity of the fuel pebbles was to be taken into account, i.e. self-shielding of the fuel grains in the fuel pebble, as well as the self-shielding of the pebbles in the lattice.

For this study, the spectrum/lattice solver embedded in PEBBED as a subroutine was run in a 'standalone' mode. For the slowing down calculation, COMBINE 7.1[8] solves the $B_1$ or $B_3$ approximations to the transport equation. COMBINE 7.0 reads 167-group data prepared from the ENDF/Bv7.0 nuclear data libraries and computed resonance absorption using Bondarenko interpolation. The Nordheim Integral Treatment can be invoked for resolved resonances. The background cross sections are adjusted for random lumping of the fuel using Dancoff factors computed using PEBDAN[9]. Infinite medium cross sections are then assigned to regions in the ANISN 1-D discrete ordinates model of the particle. The flux solution of the $S_n$ model is averaged over space to yield homogenized cross sections for the 1-D (spherical) model of the entire pebble and the process is repeated.

Of the six unit cell configurations specified in the benchmark, only the first one (LP-1) is reported here. LP-1 consists of a single moderator pebble and two identical fuel pebbles spaced such that the overall packing fraction is 0.7405. In the 1-D COMBINE-7 model, a single fuel pebble is surrounded by an extra thick graphite shell region which is sized to yield the correct overall ratio of graphite to fuel (see Figure 1).

![Fig. 1: LP Unit Cell Model (left) and the One-Dimensional COMBINE-7 Equivalent](image)

A number of participants performed the exercise using either deterministic or Monte Carlo transport codes [10], each of which read from a different set of nuclear data files (ENDF/B3,4,5, JEF1,2 or combinations thereof).

Table 2 shows the minimum, mean, and maximum of the reported results along with those generated in this study using COMBINE-7.

<table>
<thead>
<tr>
<th></th>
<th>min</th>
<th>mean</th>
<th>max</th>
<th>INL</th>
</tr>
</thead>
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<td>1.6943</td>
<td>1.7184</td>
<td>1.7290</td>
<td>1.7269</td>
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<tr>
<td>$B'$</td>
<td>7.07E-4</td>
<td>7.73E-4</td>
<td>7.91E-4</td>
<td>7.80E-4</td>
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<td>$k_{B2}$</td>
<td>1.6511</td>
<td>1.6721</td>
<td>1.6883</td>
<td>1.6772</td>
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<tr>
<td>$M^2$</td>
<td>828</td>
<td>874</td>
<td>952</td>
<td>960</td>
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<td>$\rho_{28}$</td>
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<td>$\delta_{25}$</td>
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<td>$\delta_{28}$</td>
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<td>1.65E-3</td>
<td>1.85E-3</td>
<td>1.67E-3</td>
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<td>$C^*$</td>
<td>0.185</td>
<td>0.192</td>
<td>0.192</td>
<td>0.190</td>
</tr>
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</table>

Table 2: Summary of Results from LP-1 Unit Cell Calculation

It is interesting and informative, particularly for the novice analyst, to investigate the effect of different modeling approaches and options afforded by a deterministic tool such as COMBINE-7. For example, in this study three different models were constructed according to the LP-1 specification and illustrated in Figure 1. In all three, an explicit model of the TRISO fuel particle and surrounding matrix was used to generate homogenized infinite medium cross sections for the fueled region of pebble. In the first model (LP-1a in Figure 2), the three subregions (fuel, shell, and coolant) were specified as separate materials in the ANISN model. Critical leakage was simulated as a pseudo-absorption term, $DB'$, in the transport equation. The user-supplied $B'$ value was multiplied by the diffusion coefficient computed for each of the regions and adjusted to yield $k_\infty = 1$. In the second model (LP-1b), the spatial transport solution was used to homogenize the three regions. Another transport calculation was performed over the homogenized cell with the buckling multiplying the average diffusion coefficient, $D_0$, to simulate the leakage. In the third model (LP-1c), the cell was also homogenized but leakage was simulated with a vacuum boundary condition. The radius of the homogenized pebble was increased until criticality was attained.
The results are shown in Table 3. The LP-1b model was used to generate the INL values in Table 2 as this is the type of model employed in PEBBED.

<table>
<thead>
<tr>
<th></th>
<th>LP-1a</th>
<th>LP-1b</th>
<th>LP-1c</th>
<th>LP-1bc</th>
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<td>(k_{\infty})</td>
<td>1.7269</td>
<td>1.7269</td>
<td>1.7269</td>
<td>1.7269</td>
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<tr>
<td>(B^2)</td>
<td>1.43E-3</td>
<td>7.80E-4</td>
<td>7.64E-4</td>
<td>6.58E-4</td>
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<tr>
<td>(k_b)</td>
<td>1.6770</td>
<td>1.6772</td>
<td>1.6755</td>
<td>1.6819</td>
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<tr>
<td>(M^2)</td>
<td>527</td>
<td>960</td>
<td>978</td>
<td>1132</td>
</tr>
<tr>
<td>(\rho_28)</td>
<td>7.51</td>
<td>7.63</td>
<td>7.69</td>
<td>7.77</td>
</tr>
<tr>
<td>(\delta_{25})</td>
<td>0.110</td>
<td>0.110</td>
<td>0.111</td>
<td>0.112</td>
</tr>
<tr>
<td>(\delta_{28})</td>
<td>1.81E-3</td>
<td>1.67E-3</td>
<td>1.71E-3</td>
<td>1.66E-3</td>
</tr>
<tr>
<td>(C^*)</td>
<td>0.187</td>
<td>0.190</td>
<td>0.181</td>
<td>0.192</td>
</tr>
</tbody>
</table>

Table 3: Results from Different Models of the LP-1 Unit Cell

The differences are most significant between LP-1a and LP-1b. The critical buckling in LP-1a is almost double that of LP-1b and the migration area is correspondingly lower. This is important to note in PEBBED calculations as buckling terms computed from the global diffusion solution are used to adjust the infinite medium spectra for each zone. One must understand the internal leakage model used in such a code and confirm it with independent analysis. The relatively minor differences between LP-1b and LP-1c indicate that using a volumetric pseudo-absorption (\(DB^2\)) term to represent leakage is a reasonable approximation to actual surface leakage from the cell.

Pebble bed reactor neutronics veterans are familiar with the problem of inter-pebble neutron streaming. Traditional unit cell homogenization techniques do not adequately capture the streaming between randomly loaded pebbles in which 1) the mean free path is long compared to the dimensions of the coolant (void) spaces between pebbles, and 2) the shape of these spaces varies stochastically. Lieberoth [11] derived a semi-analytical correction to the diffusion coefficient that has been shown in critical experiments to improve computational predictions of critical dimensions. The correction increases the diffusion coefficient, typically by 5-15% depending upon the total cross section, pebble radius, and local packing fraction. This correction is a feature of many PBR neutronic analysis codes and is optional in COMBINE-7. To the knowledge of the authors, the treatment has not been extended to the scattering term in the neutron transport equation, thus making direct comparisons between transport and diffusion solutions somewhat difficult. In the second unit cell model (LP-1b), all leakage is captured with the \(DB^2\) term so the effect of this correction can be directly computed. The corrected indices are listed in Table 3 under LP-1bc. The critical buckling in this case is reduced by about 14%, commensurate with the increase in the diffusion coefficient.

**III.B. Comparison of 1-D Transport and Diffusion Models of Control Rods**

The control/shutdown rods in the pebble bed reactor geometries are usually located outside of the active core in the graphite reflectors. The control/shutdown rods consist of absorber material (boron carbide) sandwiched between concentric steel cylinders and suspended in the radial reflectors, usually at regular azimuthal intervals (see Figure 3).

![Fig. 3: Overhead (X-Y) View of Control Rods in the Outer Reflector](image)

Fig. 3: Overhead (X-Y) View of Control Rods in the Outer Reflector

Modeling the rods requires explicit multi-dimensional models or some sort of balanced homogenization. In many design calculations control rod have been modeled by simply smearing out the number densities or using an equivalent B-10 concentration as a gray curtain using the Method of Equivalent Cross Sections (MECS) [12],[13].

In a 2-step process similar to that used in the fuel pebbles, COMBINE-7 can explicitly model the rod in the radial dimension to account for spatial
shielding. Infinite medium fine group cross sections are obtained by adding a dilute amount of fissile material to generate a spectrum. The fine-group cross sections for the absorber region are then collapsed over the core-driven spectrum obtained from the 1-D cylindrical model core model into few-group cross sections for the diffusion model. The process was tested by comparing the results against those obtained by other transport codes. The results are also compared to those of a simplified ‘grey curtain’ model in which the number densities of the control rod (CR) region are simply smeared and inserted into the 1-D core transport model (no spatial shielding).

III.B.1 – Results of Transport Models of the Control Rod Curtain

The multiplication factor and radial flux profiles generated for the 1-D core wedge with (C1) no absorber curtain, (C2) a grey curtain with cross sections computed from smeared control rod densities, and (C3) a grey curtain with cross sections computed from a 1-D spatial model of the control rod zone. All cases were modeled with COMBINE and the XSDRN module within SCALE [14] which has a similar 1-D transport solver. Cases 1 and 2 were also solved with Serpent [15] in two dimensions such that the entire radial-azimuthal plane was modeled with reflective axial boundaries. The 2-D core plane with individual control rods was also modeled with Serpent. For the core region, the EXPLICIT option is invoked in SERPENT in which the coordinates of each of a randomly placed set of particles within the pebble are read to support exact modeling of the double heterogeneity of the fuel. Results are shown in Table 4.

<table>
<thead>
<tr>
<th></th>
<th>COMBINE</th>
<th>SERPENT</th>
<th>XSDRN</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Absorber Annulus</td>
<td>1.320810</td>
<td>1.32547 ± 3.0E-05</td>
<td>1.32275</td>
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<tr>
<td>Smeared CR Curtain</td>
<td>1.110252</td>
<td>1.12151 ± 3.5E-05</td>
<td>1.11277</td>
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<tr>
<td>Explicit 1D (r) CR Curtain</td>
<td>1.151056</td>
<td>n/a</td>
<td>1.14797</td>
</tr>
<tr>
<td>Explicit 2D (r-θ) model</td>
<td>n/a</td>
<td>1.18522 ± 3.3E-05</td>
<td>n/a</td>
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<tr>
<td>Adjusted Explicit 1D (r) CR Annulus</td>
<td>1.187174</td>
<td>n/a</td>
<td>1.18528</td>
</tr>
</tbody>
</table>

Table 4: Eigenvalues for Infinite Cylindrical Core and Reflector

The differences between $k_{eff}$ of the simple homogeneous grey curtain and that of the explicit models indicates the large amount of spatial shielding of the absorber rings of the CR annulus.

The multistage approach used in COMBINE has an extra degree of freedom; that of the amount of reflector graphite surrounding the control rod assumed in the unit cell model of the control rod region. Adjusting this has a significant impact on the spectrum within the rod. The third row of values shows the case in which the mass of graphite in the curtain was preserved. The bottom row of values shows the eigenvalues produced by COMBINE and XSDRN after adjusting the graphite radius to yield a match with the 2-D Serpent model. This adjustment changed the core eigenvalue by ~3000pcm. A rigorous method of proscribing the radius of the graphite annulus must be developed in order to use the multi-stage COMBINE approach for cores with control rods. Alternatively, a 2-D transport model of the CR region would be required to obtain a reference spectrum for the control rod in advance of the core calculation.

The thermal (G1) and fast (G2) flux profiles are important because the fine-group cross sections are collapsed into few-group structure using the final calculated spectrum. The 1D flux profiles for different cases are shown in Figure 4 - Figure 6. The flux profiles match quite well for the cases where there are no control rods and where the control rods are homogenized simply by smearing the number densities. However, when the 2-stage homogenization with graphite mass conservation is compared with the explicit modeling, the flux profiles show considerable differences. These are reduced by adjusting the graphite mass to match the Serpent spectrum (Figure 7). The flux profiles with the corrected spectrum are shown in Figure 8.
Ultimately, however, the cross sections produced in this process must yield comparable reaction rates in the full core diffusion model. The corresponding 1-D PEBBED diffusion model of the simple core with grey curtain was run with the VSOP 4-group energy structure and compared to the COMBINE discrete ordinates (Sn) solution. The control rod was modeled in 1-D with graphite mass conserved (no spectral matching). The transport and diffusion solvers produced eigenvalues of 1.202 and 1.216, respectively, a difference of about 1200 pcm. The group-wise fluxes are shown in Figure 9.

The fluxes differ by up to 5% in certain points in the core and reflector but there is good agreement across the control rod zone. Better overall agreement would be expected with a spectrum-matching model for the control rod region.
These computational exercises confirm that the embedded, multistage COMBINE-7 approach to few-group cross section generation yields results that are consistent with other codes but that a further step must be taken to obtain accurate reaction rates in a control rod region. In the following section, we use the unrefined tool to model two pebble bed critical experiments, HTR-10 and HTR Proteus.

IV. COMPARISON TO CRITICAL EXPERIMENTS

A number of critical pebble bed experiments have provided data for code validation (ASTRA, KAHTER, HTR-PROTEUS, HTR-10). The last two were chosen for this study. As PEBBED solves the diffusion equation on an orthogonal mesh, details of many core structures are lost in the homogenization process, injecting uncertainty into the result. Nonetheless, the embedded 1-D transport capability in PEBBED allows explicit treatment of many structures, mostly importantly the fuel pebbles but also certain absorber elements and some support structures. Diffusion coefficients for the gas plenum above the pebble bed are obtained using the method of Gerwin and Scherer. As the set of measurements available from these experiments is rather limited, the modeling efforts were restricted to eigenvalue and control rod worth calculations (when applicable).

IV.B. HTR-Proteus Core 4

Of the 13 core configurations mentioned in the previous section, Core 4.2 was chosen for this study as it was loaded randomly with a 50:50 mixture of graphite and fuel pebbles. To simulate the conical discharge region found in pebble bed power reactor designs, wedge-shaped graphite wedges were placed at the bottom of the core cavity. 4940 fuel pebbles (16.74% enriched uranium) were loaded with an equal number of graphite pebbles. Pebbles forming the top surface were relocated to form a relatively ‘flat’ top that was measured to be 1.52 m above the bottom of the cavity. This yields an average packing fraction of 0.599. A Peralumen structure held the top reflector in position over the core. Further details can be found in [6].

A simplified model with azimuthal symmetry suitable for application of codes such as PEBBED was developed as part of the experimental program. Many features of the actual core, including the control rods, were eliminated from this model. Measured and computed reactivity worths of the eliminated structures were provided such that the eigenvalue of the simplified model was estimated to be 1.0129.

The PEBBED model consisted of four fuel compositions: one for the pure pebble mixture and three representing a mixture of fuel pebbles, graphite pebbles, and graphite bottom wedge material in proportions that preserved the overall number densities. Graphite reflector compositions contained 1.33 ppm boron. The model also contained three top plenum compositions consisting of various proportions of moist air, graphite, and aluminum, and one concrete composition. Insofar as the aluminum structure possessed one-dimensional symmetry, COMBINE-7 1-D models were used to generate few group cross sections for these as well as the fuel pebbles as described above. The streaming correction was applied to the pebble compositions. The composition for a withdrawable control rod consisting of two concentric stainless steel tubes was created but not used in the simplified core. The PEBBED model showing the spectral nodalization is shown in Figure 10.

Although the results of the unit cell calculations (previous section) yielded good agreement with other codes and methods, capturing the eigenvalue for the full core model proved to be difficult. The PEBBED value for $k_{eff}$ is 1.0298, about 1690 pcm above the ‘critical’ eigenvalue for the simplified core. This is quite high but to some extent consistent with the results of benchmark evaluations [17]. A detailed model computed with MCNP and ENDF/Bv7.0 data yielded an eigenvalue that was about 1350 pcm higher than the experimental value. MONK results with the same model yielded values that were between 500 and 900 pcm higher than
expected. Yet another evaluation performed using MCU5 yielded an eigenvalue that was 1550 pcm high. These results indicate 1) a common bias in the models or in the experimental data, and 2) the sensitivity of the calculated eigenvalue to small differences in the models, such as assumed pebble location. Nonetheless, further effort is needed to refine the PEBBED model or otherwise ascertain the source of the uncertainty.

One source of uncertainty is the packing of the pebbles. The overall packing fraction was measured to be 0.599. The pebble placement routine used in the PEBDAN code resulted in a core average packing fraction of 0.591. More importantly, however, the spatial profile computed by PEBDAN captured the ‘wall’ effect which causes the local packing density to oscillate in the range of a few pebble diameters of the core-reflector interface.

![Fig. 11: Radial Packing Density in Proteus as Computed by PEBDAN][9]

While the local packing fraction away from the wall is roughly equal to the measured value (~0.60), over the 9.6 cm range represented by the outer core spectral zone in PEBBED the packing fraction is closer to 0.56. The PEBBED model was modified to account for this variation which has the net result of concentrating the fuel toward the interior of the core cavity and lowering the overall leakage. Indeed the new eigenvalue computed by PEBBED is 1.0354 (+2250pcm). Accounting for this phenomenon makes a poor (reactivity) result even worse but it does indicate the sensitivity of the core eigenvalue to changes in pebble location and packing.

Finally, two control rods were partially inserted into the core to achieve criticality. An automatic control rod consisting of a wedge shaped bar of copper was measured to have a worth of about -3.3E at its critical insertion and was not modeled. A withdrawable control rod consisting of concentric stainless steel tubes was measured to have a worth of -51.5E at critical insertion. The delayed neutron fraction ($\beta$) was computed to be 0.00723. This rod was modeled explicitly in PEBBED using the method described in the previous section. The core eigenvalue computed with PEBBED with this rod inserted was 35E lower than the unrodded core. Given the high error in the overall core neutron balance, high error in associated rod worth calculations comes as no surprise. A better result may also be obtained with the use of a 2D ($r$-$\theta$) transport model for spectrum matching. Nonetheless, further study is required to ascertain the sources of uncertainty and error in this calculation before the modeling method can be considered validated.

**IV.B. HTR-10 Initial Criticality**

The HTR-10 is a small (10 MWt) pebble-bed research reactor intended to develop pebble-bed HTR technology in China. It is fueled with billiard-ball-size spheres containing TRISO-coated fuel particles embedded in a graphite matrix. The core is a cylindrical cavity of 90 cm radius. For the approach to criticality, the conical region formed by the lower graphite reflector blocks was filled with pure graphite pebbles so that bottom of the active core was level with the horizontal. The active core was a mixture of graphite and fuel pebbles in a 43:57 ratio. No control rods or other absorber elements were inserted. Other details are contained in [18].

The PEBBED simplified model consisted of one (doubly heterogeneous) fuel composition, a dummy (graphite) pebble composition, two mostly gas compositions for the top plenum and riser channel, and 79 reflector compositions with densities varying from that of pure graphite derived from coolant and other holes. The streaming correction was applied to the diffusion coefficients in the fuel and dummy pebble compositions.

The core was observed to go critical upon the loading of 16890 total pebbles with absorbers neither in the core nor in the reflector. By assuming a packing fraction of 0.61, the core height was computed to be 123.06 cm. The eigenvalue computed by PEBBED for this configuration was 0.9835 (-1653 pcm). The $k_{eff}$ was then computed for various assumed core heights from which a critical height was then interpolated to 128.61 cm, corresponding to 17589 pebbles, more than actually loaded by 699 pebbles. This estimate exceeded the critical number of pebbles originally computed using other codes and modeling schemes but not by a significant amount [19]. Interestingly, the computed eigenvalue for the same model but
Once again the uniform packing assumption was relaxed. First, given the measured packing of the Proteus pebble bed, the assumed value of the overall packing density, 0.61, was decreased. Simulations of the packing of the HTR-10 core were performed by the PEBBLES and PEBDAN codes yielding core-average values of 0.581 and 0.589, respectively. A value of 0.584 was chosen for calculating Dancoff factors and nuclide densities in PEBBED. This value corresponded to a core height of 128.6 cm and the PEBBED composition mesh was adjusted accordingly. Assuming a uniform packing density throughout, PEBBED computed a core eigenvalue of 0.9897. Interpolation among cores with different heights yielded a critical height of 131.95 cm, corresponding to 17329 pebbles and error of 439 pebbles, an improvement and well within the range of values computed by the other codes.

Finally, the uniform packing assumption was relaxed. The radial packing profile computed by PEBDAN, which looks very much like that computed for Proteus (Figure 11), was used to vary the concentration of fuel in the core. The average height of 128.6 cm was maintained. The eigenvalue computed by PEBBED is 0.9925, corresponding to a height of 126.18 cm and 16571 pebbles. This error of -319 pebbles yields the best agreement yet with the experiment.

The sensitivity of the eigenvalue to pebble packing and the correction to inter-pebble streaming are both on the order of a few hundred pcm. The top cone formed by dropped pebbles was not modeled and the error introduced by this omission has also been estimated to be on the order of a few hundred pcm [21]. These are just a few of the sources of uncertainty in such a calculation; a full and proper sensitivity analysis would be required to characterize all of them. For a design codes such as PEBBED, however, errors less than 1000 pcm would not be unexpected; errors of <500 pcm can be considered small enough to be washed out by other sources that affect core temperatures, burnup, etc. Eigenvalues should be reported with the appropriate number of significant digits to reflect this.

The error observed in the HTR-Proteus calculation is not repeated in the HTR-10 assessment so the uncertainties mentioned above are only part of the story. Benchmark evaluations of Proteus suggest that the error stems from uncertainties in the rate of neutron capture in the graphite by either the boron or the carbon itself [20]. The boron concentration in Proteus and HTR-10 pebbles are about 0.4 ppm and 1.3 ppm, respectively. Likewise, the concentration in Proteus and HTR-10 reflector graphite are about 1.3 ppm and 4.8 ppm, respectively. Small changes in the assumed boron concentration will have a considerable reactivity effect.

V. SENSITIVITY OF SAFETY-SIGNIFICANT PARAMETERS

For a core designer, these results are interesting only insofar as these variables affect overall design and performance parameters. Therefore, the PBMR400 reactor designed by the Pebble Bed Modular Reactor (Pty) Company of South Africa was chosen for use in a design study. A simplified model of this reactor served as the basis of a code-to-code benchmark study coordinated by the International Atomic Energy Agency [22]. In one exercise of that benchmark, the geometry and core and fuel compositions were specified and the equilibrium power, temperature, and burnup profiles (for $k_{eff} = 1.00$) were to be computed using the participants’ own code and nuclear data libraries.

PEBBED results for this exercise were reported in [5] and were found to compare favorably to those generated by the two codes used in the original project, even though the Nordheim Integral Treatment (NIT) was not used to compute resonance absorption in that computation. In this study, PEBBED model was re-analyzed using NIT and different assumptions about neutron streaming (with or without the streaming correction) and pebble packing (uniform or variable). The maximum temperature attained after a sudden loss of forced cooling (DOFC) was also computed using the THERMIX-KONVEK code.

Case 1: Uniform packing of 0.61, streaming correction to the diffusion coefficient applied, NIT for resolved resonances of U and Pu

Case 2: Uniform packing of 0.61, streaming correction to the diffusion coefficient not applied, NIT

Case 3: Average packing of 0.599 (computed by PEBDAN) but varying radially, streaming correction to the diffusion coefficient applied, NIT
Proceedings of the HTR 2014  
Weihai, China, October 27-31, 2014  
Paper HTR2014-51253

<table>
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<tr>
<th>Parameter</th>
<th>Case 1</th>
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<th>Case 3</th>
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<td>Pebble Flow Rate (d⁻¹)</td>
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<td>Mean Discharge Burnup (MWD/kgₘₑₜ)</td>
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<td>Average Moderator Temperature (°C)</td>
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<td>Average Coolant Temperature (°C)</td>
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<td>Maximum DLOFC Temperature (°C)</td>
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<td>1740</td>
</tr>
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</table>

Table 5: Integral Core Parameters for the PBMR-400 under Different Modeling Assumptions

The uniform packing assumption leads to slightly conservative values for power peaking compared to the core with variable packing. Fuel economy (as measured by the discharge burnup of the pebbles) is also lower in the variably-packed core. Overall, however, the temperatures are not significantly different such that the packing and other parameters investigated in this study need to be included in a detailed safety analysis.

VI. SUMMARY

This study reveals some of the challenges associated with the modeling of pebble bed reactors using the multiscale, multiphysics design code PEBBED. The code exploits the considerable one-dimensional symmetry of most PBR cores with the use of online 1-D transport for homogenizing the pebbles and other structures, with transverse leakage corrections carried by buckling terms. The unit cell and 1-D models were confirmed numerically against other codes and models. Further work is needed to validate the PEBBED approach to the modeling of control rods. The modeling of critical experiments poses a particular challenge because of the geometric complexity and large amount of graphite. Reasonable results were obtained for the HTR-10 core but not so much for Proteus Core 4. Benchmark evaluations suggest that much of this error may be attributed to poor assumptions about the neutron capture rate in graphite.

Assumptions about neutron streaming between, and packing of, pebbles display reactivity effects that are significant (higher than random uncertainties) in criticality predictions but have only minor effects on safety-significant integral parameters.

This work was supported by the U.S. Department of Energy, Office of Nuclear Energy, Science, and Technology, under DOE Idaho Operations Office Contract DE-AC07-99ID13727, in support of Very High Temperature Reactor research and development.

REFERENCES


