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A COMPARISON OF PEBBLE MIXING AND DEPLETION ALGORITHMS USED IN PEBBLE-BED REACTOR EQUILIBRIUM CYCLE SIMULATION

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ABSTRACT

Recirculating pebble-bed reactors are distinguished from all other reactor types by the downward movement through and reinsertion of fuel into the core during operation. Core simulators must account for this movement and mixing in order to capture the physics of the equilibrium cycle core. VSOP and PEBBED are two codes used to perform such simulations, but they do so using different methods. In this study, a simplified pebble-bed core with a specified flux profile and cross sections is used as the model for conducting analyses of two types of burnup schemes. The differences between the codes are described and related to the differences observed in the nuclide densities in pebbles discharged from the core. Differences in the methods for computing fission product buildup and average number densities lead to significant differences in the computed core power and eigenvalue. These test models provide a key component of an overall equilibrium cycle benchmark involving neutron transport, cross section generation, and fuel circulation.

Key Words: pebble-bed, depletion, mixing, equilibrium cycle, reactivity.

1. INTRODUCTION

The Demonstration Power Plant (DPP) being developed by PBMR (Pty) Ltd. of South Africa is a 400 MW_{th} pebble-bed high temperature reactor in which spherical fuel elements (pebbles) trickle slowly through an annular vessel during power operation. Each pebble is reinserted into the core until a specified burnup target is achieved, usually after six passes. Upon reaching this target, the pebble is discharged from the core and replaced with a fresh pebble. After some months of operation, the core asymptotically approaches a configuration in which the overall power and burnup profile remains largely unchanged and the reactor is operating in a so-called equilibrium cycle [1]. As most of the operating life of the reactor is spent at equilibrium, many of the performance and licensing calculations assume this core configuration.

Simulations of the core must therefore account for the motion of pebbles and their reinsertion into the core. Both VSOP [2] and PEBBED [3] codes were designed with this functionality, but the algorithms and numerical techniques are sufficiently different as to be a source of uncertainty in burnup calculations. A rigorous benchmarking of a pebble-bed reactor (PBR) equilibrium cycle analysis would involve the validation of neutron, thermal, and mass transport phenomena. Such an analysis is currently impossible, given that no PBR has ever operated in an equilibrium cycle. Even a full code-to-code comparison is difficult because the simulation of these transport processes involves numerous methods, assumptions, and data sources, each of which is a source of uncertainty in the final result. It remains, then, to decompose the simulation into separate exercises, each capturing a small number of processes that can be simulated (and validated if data exist) with the appropriate modules within the codes in question.

Neutron transport, thermal-hydraulics, kinetics, and few-group cross section generation have been or can be addressed through other benchmark activities. This study focuses on the nuclide tracking and depletion algorithms, which are the distinctive feature of PBR fuel management codes. Profiles and microscopic cross sections of a simplified PBR core geometry with a given flux and pebble velocity provide the template for calculating burnup in the pebbles. These inputs are generated using VSOP, assuming a specified fresh fuel composition and a pebble flow rate that is adjusted to maintain a core multiplication factor of unity. The cross sections and fluxes generated by VSOP are used in PEBBED to estimate the effects of various modeling assumptions and computational techniques.

Once-through-then-out (OTTO) and multipass fuel management schemes are analyzed in this study, and the densities of selected isotopes in the discharged fuel are compared. Differences between the isotopics densities in the OTTO cycle predicted by the codes can be attributed to the technique employed to solve the Bateman equations and to different averaging techniques. Differences between the isotopic densities predicted for the multipass model can be attributed to this solution scheme, plus any discrepancies introduced by the pebble mixing algorithms.

Because isotopic depletion drives change in the core multiplication factor (k_{eff}) , the uncertainty introduced by the different depletion and mixing assumptions can be expressed as a reactivity computed from the k_{eff} values obtained from VSOP and PEBBED for the various cases. Alternatively, the overall pebble velocity can be adjusted in the PEBBED model to achieve a critical k_{eff} with consequences for overall burnup and the densities of selected isotopes.

2. ISOTOPIC DEPLETION AND PEBBLE TRACKING ALGORITHMS IN VSOP AND PEBBED

The codes compared in this study are VSOP-99/05 [4] and PEBBED, although the tests could be performed by any PBR code with fuel management capability. VSOP is the most widely used and mature code and is under development at the Jülich Research Center for the German HTR program. The code has been updated and improved [5] for the design and licensing of the DPP. VSOP is an integration of a number of legacy core analysis tools such as CITATION (neutron diffusion) and THERMIX-KONVEK (heat transfer and gas dynamics). Few group cross sections are computed from ENDF and JEF nuclear data libraries using the GAM-THERMOS sequence

with resonance integral parameters processed in advance using ZUT. Burnup calculations are enabled by a stepwise, time-dependent coupling of the diffusion and linear depletion equations using a step-wise pebble flow management scheme. This allows for the simulation of both the equilibrium cycle and the pre-asymptotic core (the so-called 'running-in' period) as well as other non-equilibrium burnup states.

PEBBED has been under development at Idaho National Laboratory since 1999 and was designed for scoping studies and core design. It solves the transmutation equations over a spatial mesh by assuming that the flux within the mesh is constant over time and therefore converges directly upon the equilibrium core configuration. Iterative steps taken toward final convergence have no physical significance. Thermal and coolant flow data are generated with THERMIX-KONVEK, and diffusion theory constants are generated online using COMBINE [6].

The pebble tracking and nuclide depletion solvers employed by these codes are discussed in more detail in the following sections.

2.1 VSOP

The current version of VSOP computes the transmutation of 28 heavy metal isotopes using an exponential matrix algorithm derived from the ORIGEN-JUEL-II code [7,8]. A transition matrix is constructed for the group of heavy metals, the size being determined by the number of isotopes defined in the material library. This library contains an identification number for each nuclide to be treated. It also contains the decay constants and information about the possible nuclide transitions by α, β^-, β^+ decay, (n,2n), and isomeric transition. According to available cross section data, the GAM library presently defines the heavy metal chain from Th-232 through Cm-244. The number of the materials in the library can be extended [8]. The burnup of 44 fission products (including a cumulative pseudo-fission product) is treated using a finite difference algorithm based upon the FEVER code [9].

The pebbles in each user-specified zone of the core and burnup stage are lumped into batches. Batch compositions are assigned to successive zones of the core to simulate, in a stepwise fashion, pebble motion along prescribed flow-lines. The flow-lines simulate the pebble movements in both the radial and axial directions (see for an example). The volume between two flow lines is divided into a number of zones of equal volume. The relative number of zones in the different flow lines determines the relative flowing speeds. Batches that are co-located in a zone define pebbles that move together, simulating the mixing of the pebbles of different burnup levels within this region, which defines a single burnup zone. Further details of the VSOP burnup algorithm are provided in Section 2.3.

2.2 PEBBED

The depletion module in PEBBED solves the Bateman equations [10] using Laplace transforms, and thus requires the linearization of the burnup chains. PEBBED currently assumes that all pebble flow is axial and thus the burnup equation can be solved over the same (R-Z) mesh as used for solving the diffusion equation. The boundary condition is the set of nuclide densities at

the top of the core (entry plane) and the depletion time step is obtained directly from the height of each node and the pebble speed through the mesh. Moving sequentially downward through each radial channel, the nuclide densities are obtained at each node boundary. Average node densities are approximated from the boundary values and used to update the solution to the diffusion equation. Because the flux profile of the equilibrium core is not known in advance, an initial guess for the profile is assumed (usually the profile of a core with all fresh fuel). The code iterates between the diffusion and depletion solvers until the overall solution converges to within a specified tolerance.

For recirculating fuel management schemes, each pebble type is subjected to this burnup calculation for every pass computed for that type. The nuclide densities at the bottom (exit plane) are computed after each pass. The exit plane values for all but the last pass are mixed along with the fresh fuel number densities to get a weighted average burnup for each channel at the entry plane. This requires an outer iterative loop, as the equilibrium flux profile is not known in advance. The exit plane and fresh pebble densities are weighted according to the flow rate into the channel and the nature of the recirculation scheme. This scheme may have a radial or burnup dependence, depending on the design of the core and fuel handling system. The weights for each pebble type, channel, and pass are computed from the core geometry, target discharge burnup, fresh fuel composition, and channel flow rates and are stored in a *recirculation matrix* [11].

The velocity of pebbles through the core is assumed to vary with the square of the distance from the center of the core. A 2^{nd} order polynomial is fitted to the assumed velocity profile and used in the calculation of the recirculation matrix elements.

PEBBED contains simple sets of nuclides and their depletion chains as options for the user. These can easily be expanded or replaced by other chains. For this study, the VSOP 80-material set of actinides and fission products were added.

2.3 Computational Flow and Averaging Considerations

VSOP employs a sequential fuel loading and burnup algorithm that is also applicable for analysis of nonequilibrium core states such as approach to criticality, the running-in phase or special cases such as short-term continual operation without refueling. By contrast, PEBBED assumes an equilibrium core at all times and iterates to a self-consistent burnup and flux solution. The requirements of the algorithms may lead to differences in the average number densities used in flux normalization. As will be shown, this accounts for some of the differences observed in the isotopics.

Assume for simplicity that the core consists of a single column of burnup zones (shown on the left in Figure 1). Each burnup zone has a unique composition with associated few-group microscopic cross sections and is updated at regular intervals. In the VSOP method, the fresh pebble composition is inserted into the top zone, burned for a specified time interval, and passed into the next zone. In the diffusion calculation the composition in the zone should represent the average composition for that volume over the defined time interval. It is therefore typically defined to be the composition half-way through the defined time interval or burnup step. This

can also be interpreted as the average composition of a layer of spheres in the middle of the zone. In a typical VSOP model, each reload burnup step is further divided into at least two substeps.

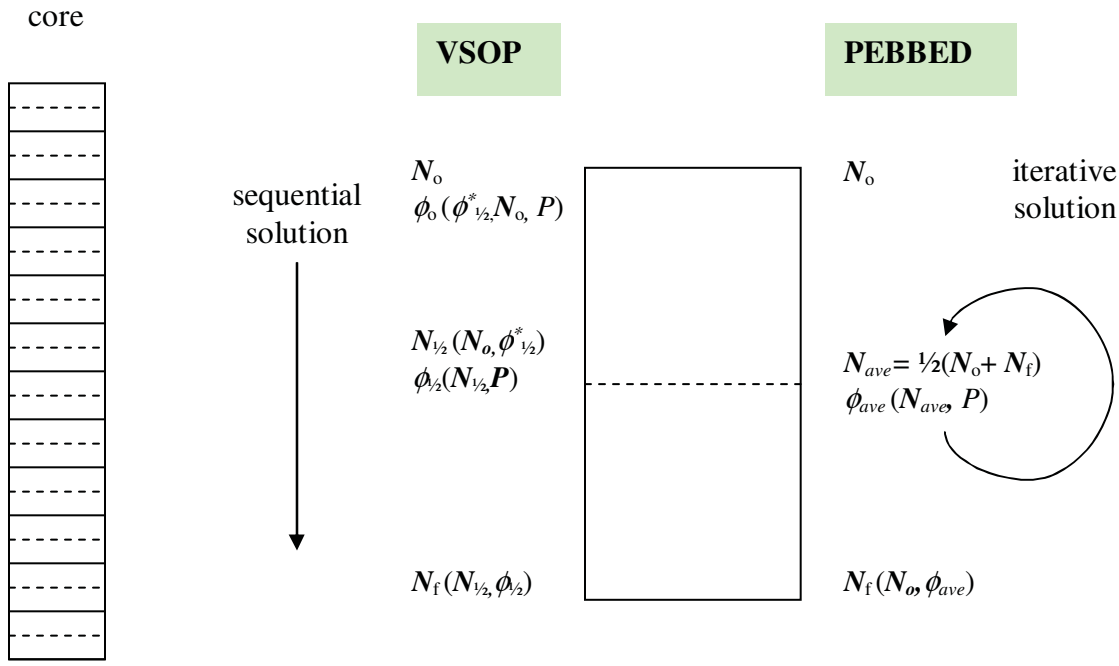

Figure 1. Single column core (left) and burnup zone.

The dashed lines in Figure 1 indicate the substeps representing the midpoint in time (averaged composition); the solid lines define the separation between zones (spectral zones) or the time at which the fuel movement takes place. In this example, there are two substeps per reload step, but the code allows any number of substeps. An even number of substeps is normally defined so that one of the time boundaries corresponds to the time midpoint (defining the average composition) before a reload or fuel movement takes place. The flux distribution and microscopic cross sections are also recalculated at this midpoint. For each substep, the flux will, however, be normalized to preserve the core total power.

At the beginning of a VSOP calculation, the burnup zones beneath the top zone are assumed to be filled with some known composition (typically graphite spheres). These spheres are replaced sequentially with the pebbles from the zone above them to simulate fuel circulation. Eventually, a critical configuration is reached and power operation can begin. When burnup calculations are performed the number densities at each substep are obtained through the end of the burnup step (bottom of the zone). Batches in the bottom zone are discarded as spent fuel or mixed with new fuel and reloaded into the top zone. This process continues at the specified input power level until the equilibrium burnup and flux solution is obtained. Note that the burnup step size (and thus the final discharge burnup) must be adjusted by user input to ensure a critical core.

Consider a single spectral zone (right side of Figure 1). In both codes, the number densities ($\boldsymbol{N}_o$) at the 'top' of the zone are known. VSOP allows the user complete freedom to select a substep (or even more than one) for which the flux shape (diffusion solution) and the microscopic cross-sections (spectrum calculation) is to be calculated and used in the burnup calculation. The input power is used to normalize this flux. For the running-in period the user can thus select the appropriate time steps (the batch composition at that time) to calculate the flux shape and cross sections to be used in the burnup calculation.

As the equilibrium cycle is reached, however, the number densities, fluxes, and cross sections at a given location do not vary (by definition of the equilibrium cycle). The following VSOP model is then typically employed. The flux profile from the previous burnup step can be used to burn the fuel through the first substep, as it should be the same as for the current time step. This flux profile normalized to the power using the given number densities $\phi_o(\phi^*_{½}, \boldsymbol{N}_o, P)$ is used to burn the isotopes in the zone from the top of the zone to the bottom of the first sub-step (middle of the zone). The number densities computed at the halfway point of each zone ($\boldsymbol{N}_{½}$) are assumed to be an approximation of the mean values for the zone and are used to calculate the new flux profile ($\phi_{½}$) and microscopic cross sections ($\sigma_{½}$). These are to be used in the second substep of the current time step and in the first substep of the next burnup step. Note that the flux ($\phi_{½}$) is re-normalized to the input power for each substep using the appropriate number densities (N_0 or $\boldsymbol{N}_{½}$). Therefore, each burnup step consists of two flux vectors, one for the first half of the burnup calculation and another for the second. The first flux vector retains the shape computed from the previous burnup step but is re-scaled to conerve core power. The densities obtained at the end of the time-step ($\boldsymbol{N}_f$) are used as the initial densities for the succeeding burnup zone, and the process is repeated until the full burnup profile of the core is obtained.

PEBBED employs a different order of operation. An initial nuclide density profile (usually all fresh fuel) is also assumed for the entire core. The core flux shape is computed and normalized to the input power. The average fluxes for each substep in the spectral zones are used to burn the fuel from the top of the zone to the bottom with the stepwise, space-dependent spectrum obtained from the diffusion solution. A full core burnup profile is computed and used to update the spectra. The code iterates between the full core burnup and flux solutions until they converge to a self-consistent solution. In contrast to VSOP, PEBBED defines the average number densities used for the flux solution to be the average of the top and bottom nuclide densities of each zone,

$$N_{ave} = \frac{N_o + N_f}{2} \qquad ..(1)$$

In order to isolate the effects of the different burnup and mixing algorithms in this study, fluxes and microscopic few-group cross sections computed by VSOP for different core models were read by PEBBED. The two flux vectors (ϕ_o and $\phi_{½}$) used in the VSOP burnup calculations were assigned to the corresponding half-step of the PEBBED burnup zones. In a modification to this approach, the linear average of the fluxes,

$$\phi_{ave} = \frac{\phi_o + \phi_{1/2}}{2}, \quad (2)$$

was also computed and used for burning over the entire spatial node corresponding to the time-step in VSOP.

There is no iteration between flux and burnup solutions in this case because the flux is not updated. However, the core power computed by PEBBED will not match that of VSOP because the VSOP flux levels $\phi_{½}$ and ϕ_o are normalized to the core power using $N_{½}$ and N_o respectively. In VSOP, these values are the closest approximation to the physical averages within the time step. If the PEBBED burnup calculation is executed using $\phi_{½}$ rather than the composite or average of ϕ_0 and $\phi_{½}$, better agreement for the core power is expected but the computed number densities would be expected to diverge. Furthermore, the half-step number densities ($N_{½}$) computed using ϕ_0 are used for the VSOP power calculation along with $\phi_{½}$. By contrast, PEBBED uses the average of the beginning and ending densities from each substep (N_{ave}) to compute the core power. These values for the average number density are not identical and thus lead to differences in the computed core power, even when the same fluxes and cross sections are used. The results given in the next section indicate a 3% difference in core power due to this effect alone when a very large time-step size is used.

Finally, the effect on core k_{eff} of these and other differences in the burnup solvers can be demonstrated by allowing PEBBED to compute the flux solution rather than using the solution from VSOP. The cross sections are still the same between the models.

3. TEST MODELS AND RESULTS

The simplified PBR core model in Figure 2 consists of a cylindrical core surrounded by a graphite reflector. For simplicity, the top gas plenum (void), loading and discharge cones, graphite inner reflector, and control elements have been omitted. The core has been (arbitrarily) divided into 5 flow channels of approximately equal cross-sectional flow area (Figure 3).

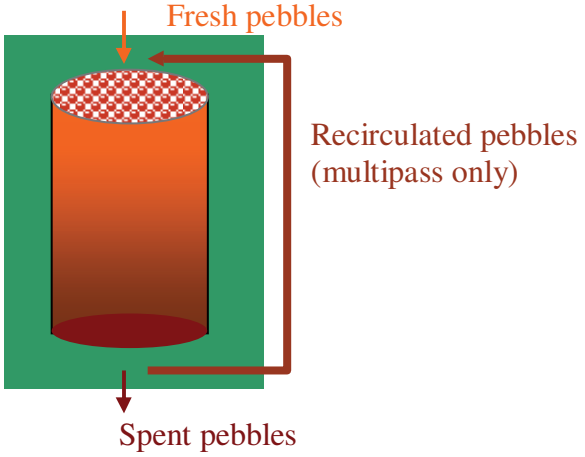

Figure 2. Simple geometry.

Figure 3. Pebble flow channels.

The active core is 10 m high and 3 m in diameter. The reflector is 1 m thick. The core is assumed to have a uniform packing density of 0.61. The fuel element design and heavy metal loading is that of the PBMR-400; each pebble has an outer diameter of 6 cm and contains ~15,000 TRISO particles dispersed in the 5 cm (outer diameter) interior region. The uranium is enriched to 9.6% U-235 and there are 9 grams of uranium in each fresh pebble. The diffusion calculations are performed using a typical VSOP 4-group energy structure (1.86 eV, 29 eV, 0.1 MeV, 10 MeV).

The first test is a simple comparison of nuclide densities after a single burnup step. Identical fluxes and cross sections are used so any observed differences can be attributed solely to the depletion algorithm employed. A short (1-day) interval and a long (89-day) interval are executed to test the treatment of short-lived isotopes in the series. For this test, a third depletion solver is also employed for comparison purposes. It is a standalone matrix exponential solver based on a Taylor series expansion. The round-off error is contained by a scaling and "time-stepping" algorithm. The maximum scaled diagonal matrix element and the maximum truncation error are specified by the user.

The second study is of an OTTO cycle. Fresh pebbles are loaded uniformly across the top of the core and discharged after passing through the core only once. To achieve an economical amount of energy from the fuel, the flow rate in OTTO fuel management schemes is necessarily slow, which also provides the necessary core residence time. This means very long burnup intervals for a core with a coarse axial mesh. For the simple core model used in this study, it takes about 188 days for a pebble to travel through a single 100 cm burnup zone. Note that such large burnup steps will typically be undesirable, since more flux normalizations are required for constant power burnup. The burnup algorithm may also require smaller burnup step sizes to avoid the numerical difficulties encountered in solving stiff systems if linear ordinary differential equations. The case was defined with simplicity in mind (to restrict the number of data sets to be shared and compared) and also to investigate these issues.

The third study is of a multipass (also known as the MEhrfachDUrchLauf or MEDUL) cycle in which pebbles discharged from the bottom are reintroduced uniformly at the top of the core for further burning.

To eliminate most sources of uncertainty, the same geometric model (discretization and boundary conditions) is used in the finite difference diffusion calculations. Though PEBBED possesses its own spectrum module, the microscopic cross sections from the converged VSOP calculation are used exclusively in the PEBBED models. Any differences observed in the results can be attributed mainly to the burnup and mixing algorithms employed. These differences would be expected to diminish with refinement of the burnup mesh; sensitivity analyses will be performed to confirm this.

3.1. Single Step Depletion Comparison

The first task in the comparison was to compare the depletion solvers directly with a single time step and common flux. Two steps (1-day and 89-day) were executed to observe the treatment of short-lived isotopes. The algorithm in VSOP checks the time-step interval against the transmutation rate constants of the individual isotopes. Sufficiently short-lived isotopes are assumed to be in equilibrium and taken out of the matrix expansion to prevent round-off error and other difficulties when manipulating rank deficient matrices. Their end-of-step densities are computed algebraically from the densities of the other nuclides. The finite difference algorithm used to compute fission product densities also assumes a linear transmutation rate over the interval. Thus, truncation errors would be expected for large time steps.

The solver in PEBBED does not make these assumptions, but it does assume that the fission yield rates of fission products are constant over the interval. Also, the linear chain solver is inherently inaccurate for long chains that loop back onto themselves. The number density of nuclide *i* in a chain is obtained by summing the contributions of its chain precursors according to

$$N_i(t) = N_i^0 \exp(-\mu_i t) + \sum_{l=1}^{i-1} \left\{ \left(\prod_{j=l}^{i-1} \xi_j \right) N_l^0 \sum_{j=l}^{i} \frac{\exp(-\mu_j t)}{\prod_{\substack{k=l \\ k \neq j}}^{i} (\mu_k - \mu_j)} \right\}, \quad (3)$$

in which

N_l^o = initial concentration of the *lth* precursor in the chain

ξ_j = link coefficient (rate at which nuclide j transmutes into nuclide $j+1$)

μ_j = loss coefficient (rate at which nuclide j is destroyed)

A singularity occurs in a loopback chain when $k = j$ so the code truncates the summation to avoid a floating point error. For example, the rate of formation of Pu-239 by the alpha decay of Cm-242 can only be approximated by PEBBED. Fortunately, such reactions are negligible in burnup calculations and can be ignored for most applications.

A significantly greater risk in solving this equation arises from numerical precision and floating point errors. Even though the equation itself is an analytic solution as opposed to a truncated expansion, its application to long chains of nuclides with widely varying transmutation rates requires the computation of products and sums with varying signs and very large exponents. The limits of floating point arithmetic in digital computers are such that significant (orders of magnitude) errors may result.

For further computational verification, results from an independent depletion solver (heretofore labeled MATRIX) were included in this single step test. As with ORIGEN, it computes a Taylor expansion of the transmutation matrix. Since the transmutation matrix was obtained from the VSOP code, the short-lived isotopes were also omitted. No subsequent equilibrium calculations were performed, so the values for these nuclides are not computed. This solver retains the full

functionality of the matrix exponential approach and uses double-precision arithmetic as opposed to the single precision used in VSOP. It is therefore used as the reference against which error is computed in VSOP and PEBBED calculations.

Table 1 shows the concentrations of nuclides in the fuel after 1 day exposure to the specified flux. Table 2 shows the concentrations after 88.972 days. In each case, all of the initial concentrations were zero except for U-234, U-235, and U-238 (1.1681E-07, 1.1936E-05, and 1.1086E-04 atoms/barn-cm, respectively). The numbers printed in *italics* were assumed to be in equilibrium and are therefore not obtained directly from the expansion of the transmutation matrix.

Table 1-A. Actinide concentrations after 1 day.

Actinide Concentrations after 1 day

	MATRIX	VSOP	% Diff	PEBBED	% Diff
TH-232	4.2465E-19	4.2465E-19	0.0%	4.2441E-19	-0.06%
TH-233		*1.9670E-24*		0.0000E+00	
PA-233	1.0877E-22	1.0875E-22	0.0%	2.2893E-23	-79%
U-233	3.0400E-16	3.0400E-16	0.0%	0.0000E+00	-100%
U-234	1.1662E-07	1.1662E-07	0.0%	1.1662E-07	0.00%
U-235	1.1880E-05	1.1880E-05	0.0%	1.1880E-05	0.00%
U-236	1.0463E-08	1.0463E-08	0.0%	1.0457E-08	-0.06%
U-237	6.6842E-12	6.6842E-12	0.0%	2.9909E-12	-55%
U-238	1.1084E-04	1.1084E-04	0.0%	1.1084E-04	0.00%
U-239		*5.2040E-10*		5.2044E-10	
NP-237	2.9597E-13	2.9597E-13	0.0%	1.0327E-13	-65%
NP-238	3.5943E-16	3.5943E-16	0.0%	8.3000E-17	-77%
NP-239	1.8694E-08	1.8694E-08	0.0%	1.8695E-08	0.00%
NP-240		*1.2229E-12*		1.1553E-12	
PU-238	3.8881E-17	3.8881E-17	0.0%	5.5021E-18	-86%
PU-239	2.8569E-09	2.8569E-09	0.0%	2.8566E-09	-0.01%
PU-240	1.8387E-11	1.8386E-11	0.0%	1.8382E-11	-0.02%
PU-241	9.0115E-14	9.0115E-14	0.0%	9.0099E-14	-0.02%
PU-242	9.3687E-17	9.3687E-17	0.0%	9.3679E-17	-0.01%
PU-243	2.5109E-20	2.5109E-20	0.0%	2.5106E-20	-0.01%
AM-241	2.7590E-18	2.7590E-18	0.0%	2.7584E-18	-0.02%
AM-242M	1.1714E-21	1.1714E-21	0.0%	1.1628E-21	-0.73%
AM-242	5.2304E-21	5.2304E-21	0.0%	5.2294E-21	-0.02%
AM-243	1.4255E-20	1.4255E-20	0.0%	1.3423E-20	-5.8%
AM-244	6.4498E-24	6.4014E-24	-0.7%	5.2147E-24	-19%
CM-242	7.2990E-22	7.2987E-22	0.0%	7.4518E-22	2.1%
CM-243	4.0999E-26			3.1344E-24	7545%
CM-244	1.3687E-24	1.3954E-24	2.0%	7.6703E-21	560309%

Table 1-B. Fission product concentrations after 1 day.

	MATRIX	VSOP	% Diff	PEBBED	% Diff
XE-135	1.7531E-10	1.7483E-10	-0.27%	1.7527E-10	-0.03%
FP44	4.3722E-08	4.3728E-08	0.01%	4.3642E-08	-0.18%
XE-136	5.4633E-09	4.2510E-09	-22%	5.4534E-09	-0.18%
KR-83	2.4462E-10	2.4465E-10	0.01%	2.4427E-10	-0.14%
ZR-95	2.9678E-09	2.9682E-09	0.02%	2.9631E-09	-0.16%
MO-95	1.5882E-11	1.5845E-11	-0.23%	1.5847E-11	-0.22%
MO-97	2.7495E-09	2.7499E-09	0.02%	2.7449E-09	-0.17%
TC-99	2.8264E-09	2.8268E-09	0.02%	2.8214E-09	-0.18%
RU-101	2.3298E-09	2.3301E-09	0.01%	2.3256E-09	-0.18%
RU-103	1.4363E-09	1.4365E-09	0.01%	1.4330E-09	-0.23%
RH-103	1.2631E-11	1.2578E-11	-0.42%	1.2594E-11	-0.29%
RH-105	3.6519E-10	3.6530E-10	0.03%	3.6395E-10	-0.34%
PD-105	9.1940E-11	8.4416E-11	-8.2%	9.1560E-11	-0.41%
PD-108	3.3216E-11	3.3221E-11	0.02%	3.2705E-11	-1.5%
AG-109	1.4074E-11	1.4076E-11	0.01%	1.3759E-11	-2.2%
CD-113	4.7487E-12	4.7500E-12	0.03%	4.7318E-12	-0.36%
I-131	1.2523E-09	1.2525E-09	0.02%	1.2503E-09	-0.16%
XE-131	5.4598E-11	5.3782E-11	-1.5%	5.4473E-11	-0.23%
XE-133	2.9310E-09	2.9316E-09	0.02%	2.9262E-09	-0.17%
CS-133	1.9683E-10	1.9244E-10	-2.2%	1.9638E-10	-0.23%
CS-134	7.2662E-14	9.7870E-14	35%	7.2388E-14	-0.38%
PR-141	2.7184E-09	2.7188E-09	0.01%	2.7139E-09	-0.16%
PR-143	2.6840E-09	2.6844E-09	0.02%	2.6798E-09	-0.16%
ND-143	6.9113E-11	6.8463E-11	-0.94%	6.8960E-11	-0.22%
ND-144	2.5163E-09	2.5167E-09	0.01%	2.5122E-09	-0.16%
ND-145	1.8142E-09	1.8144E-09	0.01%	1.8113E-09	-0.16%
ND-146	1.3805E-09	1.3807E-09	0.02%	1.3781E-09	-0.17%
PM-147	1.0445E-09	1.0446E-09	0.01%	1.0427E-09	-0.17%
PM-148M	1.0433E-12	9.9200E-13	-4.9%	1.0406E-12	-0.26%
PM-148	1.1864E-12	1.1387E-12	-4.0%	1.1813E-12	-0.43%
SM-147	3.8027E-13	3.7963E-13	-0.17%	3.7939E-13	-0.23%
SM-148	5.7747E-14	8.1277E-14	41%	5.7436E-14	-0.54%
PM-149	4.2925E-10	4.2940E-10	0.03%	4.2861E-10	-0.15%
SM-149	5.9866E-11	5.2550E-11	-12%	5.9739E-11	-0.21%
SM-150	1.1279E-11	1.3795E-11	22%	1.1250E-11	-0.25%
PM-151	1.4632E-10	1.4637E-10	0.04%	1.4603E-10	-0.20%
SM-151	4.6271E-11	4.1790E-11	-10%	4.6145E-11	-0.27%
SM-152	1.2536E-10	1.2561E-10	0.20%	1.2509E-10	-0.21%
EU-153	7.5310E-11	7.5323E-11	0.02%	7.5120E-11	-0.25%
EU-154	1.4436E-13	1.4423E-13	-0.09%	1.4315E-13	-0.84%
EU-155	1.5039E-11	1.5041E-11	0.01%	1.4987E-11	-0.34%
GD-155	7.5090E-15	7.2794E-15	-3.1%	7.4767E-15	-0.43%
GD-156	6.4767E-12	6.4766E-12	0.00%	6.4442E-12	-0.50%
GD-157	2.2340E-12	2.2347E-12	0.03%	2.2196E-12	-0.64%

The actinide data in Table 1-A indicate excellent agreement between the VSOP solver and the independent matrix exponential solver. The only noticeable percent errors are in Cm-244 and Am-244. As both of these isotopes have negligible concentrations (~1E-24 atoms/bn-cm), these can be attributed to machine precision error. The PEBBED solver shows reasonable agreement for the major actinides and can therefore be expected to yield comparable fuel burnup results. For low concentration ($<10^{-12}$ atoms/bn-cm) minor actinides, the differences range from a few percent to many orders of magnitude. While neutronically negligible in the context of core design and burnup analysis, care should be taken when using PEBBED for predictions of minor actinide content in spent fuel, such as in reprocessing or repository source terms.

Table 1-B shows that both solvers yield reasonable results for short term build-up of most fission products with errors on the order of a percent in most cases. In VSOP, Xe-135 is assumed to be in equilibrium. Its concentration is not computed by the matrix solver but directly from the fission rate. Tables 2-A and 2-B show the same results for a single burnup step of 88.972 days.

Table 2-A. Actinide concentrations after 89 days.

	MATRIX	VSOP	% Diff	PEBBED	% Diff
TH-232	2.8697E-15	2.8697E-15	0.0%	2.9278E-15	2.0%
TH-233		*1.3293E-20*			
PA-233	2.9040E-16	2.9040E-16	0.0%	2.4585E-16	-15%
U-233	2.0181E-14	2.0181E-14	0.0%	0.0000E+00	-100%
U-234	1.0093E-07	1.0093E-07	0.0%	1.0074E-07	-0.18%
U-235	7.8433E-06	7.8433E-06	0.0%	7.8069E-06	-0.46%
U-236	7.4075E-07	7.4075E-07	0.0%	7.4676E-07	0.81%
U-237		*4.1731E-09*		3.9191E-09	
U-238	1.0890E-04	1.0889E-04	0.0%	1.0887E-04	-0.02%
U-239		*5.1128E-10*		5.1121E-10	
NP-237	1.6773E-08	1.6773E-08	0.0%	1.5591E-08	-7.0%
NP-238		*1.7489E-10*		1.5204E-10	
NP-239		*7.3672E-08*		7.1981E-08	
NP-240		*4.8192E-12*		4.7086E-12	
PU-238	1.6646E-09	1.6645E-09	0.0%	1.3235E-09	-20%
PU-239	7.7554E-07	7.7554E-07	0.0%	7.8097E-07	0.70%
PU-240	2.5756E-07	2.5756E-07	0.0%	2.5393E-07	-1.4%
PU-241	1.1149E-07	1.1149E-07	0.0%	1.0752E-07	-4%
PU-242	1.3739E-08	1.3739E-08	0.0%	1.2868E-08	-6%
PU-243		*9.0556E-12*		8.3923E-12	
AM-241	3.2335E-10	3.2335E-10	0.0%	3.0444E-10	-6%
AM-242M	6.4222E-12	6.4222E-12	0.0%	5.9805E-12	-7%
AM-242		*3.5829E-12*		3.2723E-12	
AM-243	6.0555E-10	6.0555E-10	0.0%	5.4682E-10	-10%
AM-244		*1.3943E-12*		1.2233E-12	
CM-242	6.2344E-11	6.2344E-11	0.0%	5.5095E-11	-12%
CM-243	3.8629E-13	3.8629E-13		3.3016E-13	-15%
CM-244	3.8123E-11	3.8123E-11	0.0%	3.2472E-11	-15%

Table 2-B. Fission product concentrations after 89 days.

	MATRIX	VSOP	% Diff	PEBBED	% Diff
XE-135	1.6745E-10	1.7325E-10	3.5%	1.7527E-10	5%
FP44	3.9823E-06	3.8867E-06	-2.4%	3.9225E-06	-1.5%
XE-136	5.0328E-07	3.7162E-07	-26%	5.0459E-07	0.26%
KR-83	1.8825E-08	1.8391E-08	-2.3%	2.0492E-08	8.9%
ZR-95	1.6317E-07	1.6031E-07	-1.8%	1.7247E-07	5.7%
MO-95	8.9887E-08	7.4716E-08	-17%	9.4430E-08	5.1%
MO-97	2.3991E-07	2.3415E-07	-2.4%	2.4641E-07	2.7%
TC-99	2.4249E-07	2.3676E-07	-2.4%	2.4633E-07	1.6%
RU-101	2.0905E-07	2.0406E-07	-2.4%	2.0725E-07	-0.86%
RU-103	7.1681E-08	7.0794E-08	-1.2%	6.2472E-08	-13%
RH-103	6.5674E-08	4.8376E-08	-26%	5.6662E-08	-14%
RH-105	1.3514E-09	1.3936E-09	3.1%	8.7941E-10	-35%
PD-105	5.6759E-08	2.8257E-08	-50%	3.5317E-08	-38%
PD-108	1.6316E-08	1.5929E-08	-2.4%	2.8772E-09	-82%
AG-109	9.0425E-09	8.8199E-09	-2.5%	1.1535E-09	-87%
CD-113	2.5441E-11	2.6205E-11	3.0%	1.4533E-11	-43%
I-131	1.5132E-08	1.5352E-08	1.5%	1.5167E-08	0.23%
XE-131	9.6837E-08	5.3518E-08	-45%	9.4021E-08	-3%
XE-133	2.2392E-08	2.2867E-08	2.1%	2.3465E-08	5%
CS-133	2.4305E-07	1.2869E-07	-47%	2.4540E-07	0.97%
CS-134	8.1419E-09	4.4052E-09	-46%	8.2202E-09	0.96%
PR-141	2.3566E-07	2.3002E-07	-2.4%	2.4297E-07	3.1%
PR-143	4.8911E-08	4.9138E-08	0.47%	5.2406E-08	7.1%
ND-143	1.6879E-07	1.0150E-07	-40%	1.7666E-07	4.7%
ND-144	2.3023E-07	2.1946E-07	-4.7%	2.4394E-07	6.0%
ND-145	1.5125E-07	1.4767E-07	-2.4%	1.5856E-07	4.8%
ND-146	1.2392E-07	1.2085E-07	-2.5%	1.2865E-07	3.8%
PM-147	7.2590E-08	7.1074E-08	-2.1%	7.4643E-08	2.8%
PM-148M	5.1369E-10	2.5853E-10	-50%	5.2725E-10	2.6%
PM-148	7.0510E-10	3.5678E-10	-49%	7.2332E-10	2.6%
SM-147	2.4415E-09	2.1299E-09	-13%	2.4998E-09	2.4%
SM-148	4.7062E-09	2.3787E-09	-49%	4.8202E-09	2.4%
PM-149	2.1869E-09	1.7213E-09	-21%	2.2535E-09	3.0%
SM-149	1.3247E-09	5.2294E-10	-61%	1.3615E-09	2.8%
SM-150	4.8665E-08	1.1414E-08	-77%	4.8422E-08	-0.50%
PM-151	3.4598E-10	3.5692E-10	3.2%	3.2624E-10	-5.7%
SM-151	4.8459E-09	2.1342E-09	-56%	4.5046E-09	-7.0%
SM-152	2.3225E-08	1.3626E-08	-41%	2.0608E-08	-11%
EU-153	1.2121E-08	9.6779E-09	-20%	1.0457E-08	-14%
EU-154	1.4566E-09	1.1435E-09	-21%	1.2488E-09	-14%
EU-155	9.6428E-10	9.0069E-10	-6.6%	6.5629E-10	-32%
GD-155	6.1447E-12	3.0053E-12	-51%	4.1220E-12	-33%
GD-156	2.7718E-09	2.3335E-09	-16%	1.5721E-09	-43%
GD-157	1.3068E-11	1.2924E-11	-1.1%	5.3282E-12	-59%

Again the minor actinide results from the VSOP solver agree well with the MATRIX solver. The results from the chain solver in PEBBED diverge from the MATRIX results for many of the minor actinides. The error in major actinides are still small enough to allow for reasonable

burnup assessments, but care should be taken if simulating very high (>100 MWD/kg) burnup fuel cycles.

Interestingly, the performance of the codes in predicting fission product buildup is comparable. VSOP results compare favorably with the MATRIX solver for many of the direct fission products (Xe through Cd), but the code underestimates the buildup of the Sm and Pm isotopes. PEBBED shows much better agreement with Pm and Sm, but has some difficulty with Ru, Rh, and Pd. Both have difficulty with the Eu and Gd isotopes at the end of the long fission product series.

A sensitivity study was performed with PEBBED to determine if error is a strong function of the duration of the time-step. The 89-day interval was subdivided into smaller equivalent substeps with the same flux. A sample of the results after the full 89-day interval are shown in Figure 4.

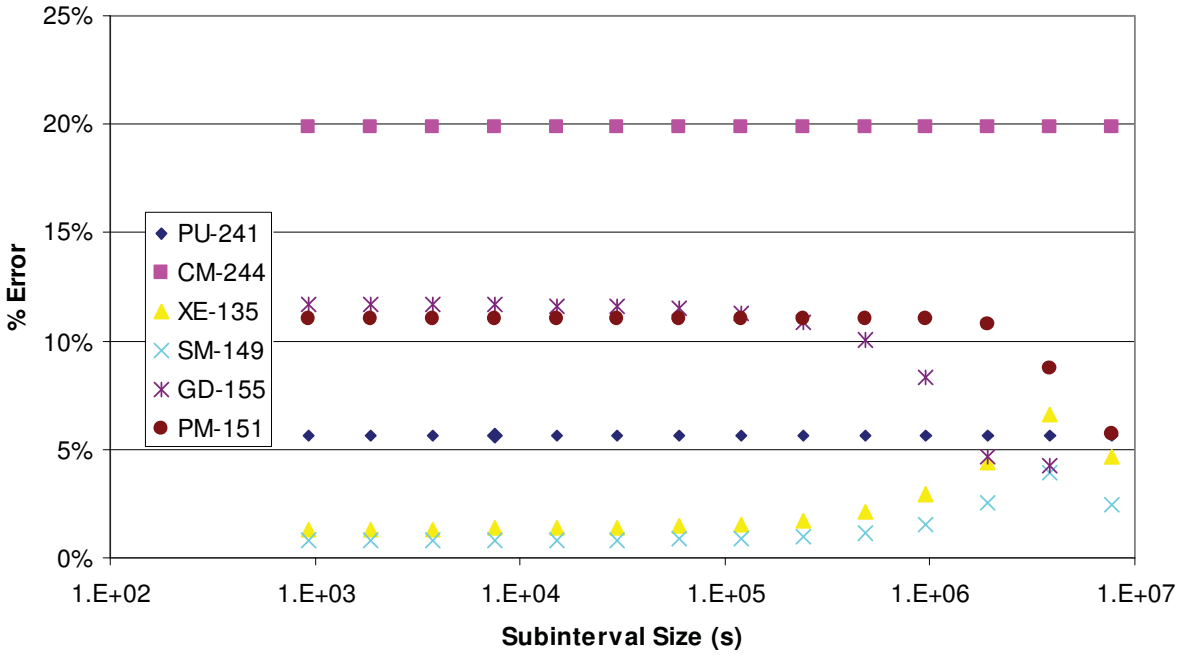

Figure 4: Percent error in PEBBED (relative to the MATRIX solution) vs. the duration of the subinterval of the 89-day burnup step.

The results are mixed but appear to fall into one of three trends. The actinides, as represented by Pu-241 and Cm-244, do not appear to be sensitive to the size of the time step; the error is quite invariant over the range. Some of the fission products (e.g. Xe-135 and SM-149) have errors, which decline to a percent or two if the substep duration is reduced to 10^5 seconds or less. Others, such as Pm-151 and Gd-155, do better with the longer substep interval.

A similar calculation was performed with VSOP, which uses a finite difference solver for the fission product chains. It is expected that the error would diminish with smaller step sizes, and it appears that a step size of less than 10^6 seconds (about 10 days) reduces the error to acceptable levels for all isotopes not assumed to be in equilibrium. In VSOP, the concentration of Xe-135 is assumed to be in equilibrium and thus it is calculated independently of the matrix solver. Changing the time-step size will have no effect on this value, as seen in Figure 5.

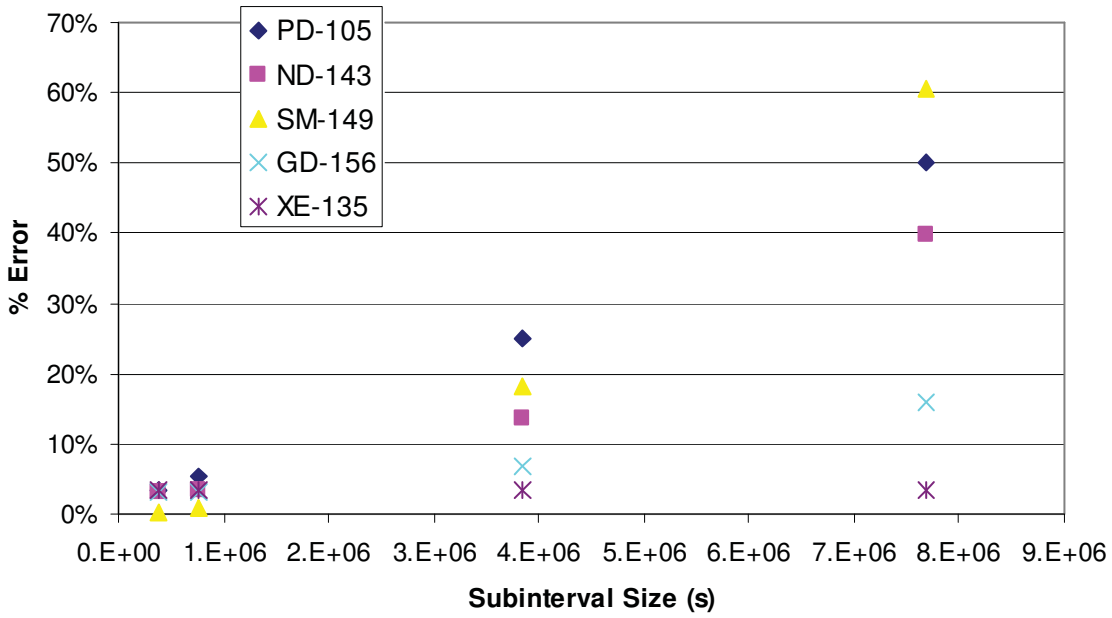

Figure 5: Percent error in VSOP (relative to the MATRIX solution) vs. the duration of the substep of the 89-day burnup step.

The matrix exponential solver used to compute the actinide concentrations in VSOP possesses an internal time-step controller and can thus accommodate an arbitrary external time-step specification without significant numerical degradation.

One aspect that was not investigated is the number of flux re-normalizations needed or the step-size sensitivity when burnup is performed at constant power opposed to the constant flux assumption made in the cases above. In VSOP the flux re-normalization is performed at each sub-step and thus the user can assure burnup error minimization by defining more sub-steps. In PEBBED, the flux is re-computed and re-normalized after each burnup sweep.

3.2. OTTO Cycle

3.2.1. Specifications and Results for a OTTO Fuel Management Scheme

The fresh fuel composition was provided in the previous section. The other parameters needed for the comparison are the radial dimensions of the five flow channels and the rate at which pebbles flow downward in these channels. The flow speed through the core is assumed to be radially uniform (slug flow). In actual pebble bed reactors, this assumption fails near the reflector boundaries as drag impedes pebble motion. Both VSOP and PEBBED allow for radially varying pebble flow rates, but accounting for this phenomenon may mask differences caused by the burnup solvers without contributing to an understanding of those differences. The channel data are given in Table 3.

Table 3. Flow channel dimensions and speeds (OTTO).

	1	**2**	**3**	**4**	**5**
Outer boundary radius (cm)	60	90	120	135	150
Speed & Flow					
- (cm/day)	0.56	0.56	0.56	0.56	0.56
- (pebbles/day)	34	43	60	36	41

Because pebbles in different flow channels are subjected to different spectra, the burnup they accrue passing through the core will vary with radial position. Table 4 reveals the variation for one of the isotopes, U-235. The fluxes and microscopic cross sections from VSOP were used in the PEBBED calculation so that any differences can be attributed to the depletion and nuclide averaging algorithms employed.

The VSOP model was chosen as the reference case (case O1) against which various PEBBED models were compared. Section 2.3 discusses the differences in the way that VSOP and PEBBED computes zone-wise nuclide concentrations. In cases O2 and O3 different flux vectors computed by VSOP were read by PEBBED along with the VSOP microscopic cross sections. In cases O3 and O4, the flux solver in PEBBED was used to compute burnup. In all cases, the same microscopic cross sections from VSOP were used. These cases are as follows:

Case O1: VSOP reference (critical core with a nominal pebble flow rate of 214 pebbles per day).

Case O2: PEBBED depletion was performed using the few-group fluxes from VSOP and the nominal core pebble flow rate of 214 pebbles per day. The calculations are performed using either a composite flux (ϕ_o) for the top half of each zone and ($\phi_{1/2}$) for the bottom half (Case O2a) or an average of the two fluxes (ϕ_{ave}) for the full zone (Case O2b).

Case O3: Same as Case O2 but the second half-step fluxes ($\phi_{1/2}$) from VSOP were used in the PEBBED burnup calculation rather than composite or average.

Case O4: is the same as Case O2 but the fluxes were computed with the PEBBED diffusion solver.

Case O5: is the same as Case O4 but the pebble flow rate was adjusted to 234 pebbles per day to obtain a critical core. The values represent flow-weighted averages over the five flow channels.

Table 4 shows the average U-235 density in the discharged fuel as computed by VSOP (case O1) and PEBBED (case O2b).

Table 4. Variation in U-235 discharge concentration (atoms per barn-cm) in the critical OTTO core (and % deviations from the mean)

	Channel 1	Channel 2	Channel 3	Channel 4	Channel 5
VSOP	2.07E-06 (-6.0%)	2.28E-06 (3.5%)	2.45E-6 (11.%)	2.29E-6 (3.7%)	1.81E-6 (-18.%)
PEBBED*	2.07E-6 (-6.0%	2.82E-6 (3.5%)	2.44E-6 (11%)	2.28E-6 (3.6%)	1.81E-6 (-18.%)

* Corresponds to Case O2b

The deviation from the mean of the channel-averaged discharge concentration is as high as 18% (Channel 5) and is due to the flux variations in the radial direction. Good agreement is observed between VSOP and PEBBED.

The transmutation of different isotopes was further studied. A few uranium and plutonium isotopes were chosen because they dominate the burnup characteristics of the pebble. Am-244 was chosen because it is a result of a longer and more complex series of transmutations among the actinides that may not be satisfactorily captured in the simple PEBBED burnup chains. Xe-135 is a direct fission product with a strong reactivity effect and Gd-155 comes toward the end of a long series of fission product transmutations.

Table 5 lists the discharge concentrations of specific nuclides as computed in the various cases.

Table 5. Comparison of average isotopic inventory (atoms per barn-cm) in discharged pebbles (OTTO) and percent differences with the VSOP result.

	U-235	U-238	Pu-239	Pu-241	Am-244	Xe-135	Gd-155
Case O1 (VSOP reference)	2.21E-06	1.04E-04	7.01E-07	3.01E-07	1.93E-14	2.14E-13	2.03E-09
Case O2 a) PEBBED with composite flux	2.21E-06 (0.0%)	1.04E-04 (0.0%)	6.90E-07 (-1.6%)	2.94E-07 (-2.1%)	1.85E-14 (-3.7%)	2.04E-13 (-4.7%)	2.39E-09 (17.8%)
b) PEBBED with average flux	2.20E-06 (0.0%)	1.04E-04 (0.0%)	6.90E-07 (1.7%)	2.94E-07 (-2.4%)	1.77E-14 (-8.3%)	2.00E-13 (-6.5%)	2.39E-09 (17.9%)
Case O3 PEBBED with half-step flux	2.03E-06 (7.9%)	1.04E-04 (-0.3%)	6.87E-07 (2.1%)	2.97E-07 (-1.1%)	2.09E-14 (8.7%)	2.04E-13 (-4.7%)	2.54E-09 (26.%)
Case O4 PEBBED with PEBBED flux, nominal flow rate	2.08E-06 (-5.5%)	1.04E-04 (-0.1%)	7.02E-07 (0.2%)	3.02E-07 (-0.5%)	1.24E-14 (-35%)	1.39E-13 (-35%)	2.56E-09 (26.%)
Case O5 PEBBED with PEBBED flux, critical flow rate	2.32E-06 (5.0%)	1.05E-04 (0.3%)	6.90E-07 (-1.6%)	2.99E-07 (-0.5%)	1.03E-14 (-46%)	1.43E-13 (-33.%)	2.25E-09 (-11.%)

The differences between Cases O1 and O2 are due entirely to the burnup algorithms. The major actinides agree for the most part but the differences between the minor actinides and some fission products are consistent with those observed in the single step tests of the previous section. The differences in actinide transmutation led to a drop in the discharge burnup from the VSOP value of 97.9 to 97.1 MWD/kg_{hm} for PEBBED Case O2.

There is no consistent bias in the differences between PEBBED and VSOP; deviations range from -46% to +26% for some of the low concentration actinides and fission products.

The results from Case O3 indicate the considerable effect of using the same (half-step) flux for the burnup calculation in PEBBED rather than using the average of the two half-step flux values. In Case O2, a composite or an average of these two flux values were used in the PEBBED calculation. This led to reasonable agreement for the discharge isotopics but the core power computed by PEBBED (189 MW) was considerably lower than that used for flux normalization in VSOP (200 MW). For better power agreement, the second half-step flux vector corresponds to the VSOP half-step number density vector and is therefore the appropriate choice. For Case O3, PEBBED computed a core power of 195 MW. This 2.9% difference is attributable to the different ways in which VSOP and PEBBED compute core fission power. In PEBBED, the total fission power is computed by summing the products of the macroscopic cross section, flux, and energy per fission for the given zone. In VSOP, a weighted average of individual nuclide energies per fission is computed and multiplied by the total fission rate (flux times macroscopic cross section). The average number densities of the previous (sub) step, however, are used for this weighting rather than those of the current step. In other words, when the fluxes are

normalized at time $t_{1/2}$, the macroscopic cross sections used for computing fission power correspond to $N_{1/2}$, but average energy per fission values correspond to $0.5*(N_0 + N_{1/2})$.

The other, and probably more significant, source is the difference in the ways that VSOP and PEBBED compute the average nuclide densities in the burnup zones (see Section 2.3). The average density of U-235 in the first burnup zone as computed by PEBBED is 0.8% lower than the VSOP value. The average density of Pu-239 in this zone computed by PEBBED is 12% lower than the corresponding VSOP value. PEBBED also computed a discharge burnup of 100.3 MWD/ kg_{hm}, 2.5 % higher than VSOP.

The differences between Cases O1, O4, and O5 show the additional effect caused by the feedback through the diffusion calculation. The flow rate of pebbles through the core was adjusted to yield a k_{eff} value of 1.0 in the VSOP model. Using the same flow rate and cross sections, PEBBED computed a k_{eff} value of 0.9914, a drop of about 860 pcm. To some extent the differences can be attributed to the diffusion solver, but a recent study (PBMR Benchmark Report comparing keff results among various codes using the same geometry and cross sections indicates that this difference accounts for no more than 200 pcm. The remaining 660 pcm is a result of the differences in burnup. Table 2-A indicates that, at least for large timesteps, the large deviations between VSOP and PEBBED occur in the minor actinides that originate from Pu-241. Case O4 was repeated but with the links from Pu-241 to these nuclides broken. The resulting k_{eff} was computed to be 0.9953, a difference of about 470 pcm. The contribution of the minor actinide deviations on the total difference is about 390 pcm. The remaining 270 pcm can be attributed to the differences in fission product buildup predicted by the codes.

Total Difference (pcm):	860
- due to diffusion solver:	200
- due to minor actinides	390
- due to fission products	270

In Case O5, the flow rate in PEBBED was allowed to increase to yield a critical eigenvalue. Fresh fuel must be added at a higher rate and spent fuel discharged earlier to counteract the higher poisoning predicted by PEBBED. The net result is a drop in the discharge burnup from the VSOP-generated value of 94.0 to 87.7 MWD/ kg_{hm}.

3.3. Multipass Cycle

In the multipass or MEDUL scheme, pebbles enter the core at the top, pass through the core, and are returned to the top of the core numerous times depending on the desired target burnup and overall pebble flow rate. The pebbles from all but the last pass are distributed randomly over the pebble-bed surface with the fraction going to each flow channel determined by the flow rate through that channel. In this model, the pebble circulation rate was increased so that each pebble passes through the core multiple times before discharge. This is controlled in PEBBED by adjusting the overall pebble flow rate; it is controlled in VSOP by changing the duration of the burnup step. Given the same discretization as in the OTTO mode, the burnup intervals are reduced by a factor approximately equal to the total number of passes as shown in Table 6. The factor only approximates the number of passes because the mixing and recirculation of pebbles

leads to a slightly more efficient utilization of fuel. Consequently the pebbles can be burned to a slightly higher level before discharge while sustaining a critical configuration. Differences due to a discretization error in the matrix solver would be expected to decline because of the smaller time-step size if the spatial mesh is not properly converged, but this may be offset to a degree by the error induced by the mixing calculation itself.

Table 6. Pebble flow rates by channel (multipass).

	1	2	3	4	5
Speed & Flow					
- (cm/day)	0.56	0.56	0.56	0.56	0.56
- (pebbles/day)	193.2	241.7	338.2	205.2	229.4

3.3.1. Specifications

The core thermal power (200 MW) and core dimensions are the same as those used in the OTTO cycle. Once again, the pebble flow rate is assumed to be uniform in the radial direction. Although the flux still varies significantly along the radial dimension, the random distribution of recirculated pebbles over the top of the core means that the burnup at the core top is constant over time and $\vec{r}$. Differences observed in the burnup of discharged pebbles in the different channels are due to the nonuniform burning of pebbles during the last pass only.
A set of cases similar to those in the OTTO study were performed with this core:

Case M1: VSOP reference (critical core with a nominal pebble flow rate of 1448 pebbles per day).
Case M2: PEBBED depletion was performed using the few-group fluxes from VSOP and the nominal core pebble flow rate of 1448 pebbles per day. The calculations are performed using the average of the two VSOP time-step fluxes for the full zone.
Case M3: Same as Case M2 but the second half-step fluxes ($\phi_{1/2}$) from VSOP were used in the PEBBED burnup calculation rather than composite or average.
Case M4: Is the same as Case M2 but the fluxes were computed with the PEBBED diffusion solver.
Case M5: Is the same as Case M4 but the pebble flow rate was adjusted to 1280 pebbles per day to obtain a critical core. The values represent flow-weighted averages over the five flow channels.

3.3.2. Results

Table 7 shows the radial variation in the discharge concentration of U-235. This variation is much lower than that computed in the OTTO case (see Table 4). As mentioned previously, the pebbles of different burnup levels are distributed evenly across the top of the core (see Table 8). Thus any differences in are the result of the burnup accrued only during the 6th pass. On the other hand, the radial concentration profiles between VSOP and PEBBED agree very well for the OTTO case, while differences are evident in the MEDUL case.

Table 7. Variation in U-235 discharge concentration (atoms per barn-cm) in the critical Multi-pass core (and % deviations from the mean)

	Channel 1	Channel 2	Channel 3	Channel 4	Channel 5
VSOP	1.62E-06 (-1.0%)	2.28E-06 (0.7%)	2.45E-6 (2.0%)	2.29E-6 (0.9%)	1.81E-6 (-3.6%)
PEBBED*	2.10E-6 (-1.8%	2.14E-6 (0.03%)	2.17E-6 (1.8%)	2.16E-6 (1.3%)	2.09E-6 (-2.3%)

* Corresponds to Case M2

Table 8 shows the burnup levels of pebbles discharged from different radial zones in the OTTO and MEDUL cores. Note the relative peaking of burnup in the OTTO vs. the multi-pass cases. Note also the accentuated peaking of the PEBBED multi-pass results compared to the VSOP results. The radially-averaged discharge burnup values agree but the distribution is considerably different even though the same flux profile was used.

Table 8. Variation in discharge burnup (MWD/kg of heavy metal) by radial channel.

	Channel 1	Channel 2	Channel 3	Channel 4	Channel 5	MEAN
VSOP						
- OTTO	107.	103.	96.7	92.5	91.5	97.9
- multi-pass	111.	110.	110.	109.	110.	110.
PEBBED*						
- OTTO	107.	102.	96.2	91.8	90.3	97.1
- multi-pass	111.	110.	109.	109.	110.	110.

* Corresponds to Case M2b

Table 9 shows the differences in discharge concentrations for the other nuclides for the different PEBBED cases described above.

Table 9. Comparison of isotopic inventory (grams per pebble) in discharged pebbles (Multi-pass)

	U-235	U-238	Pu-239	Pu-241	Am-244	Xe-135	Gd-155
Case M1 (VSOP reference)	1.64E-06	1.03E-04	7.50E-07	3.65E-07	6.23E-12	2.93E-11	4.44E-10
Case M2 PEBBED with average flux)	1.52E-06 (-7.5%)	1.03E-04 (-0.1%)	7.19E-07 (-4.1%)	3.34E-07 (-8.3%)	4.48E-12 (-28.%)	2.56E-11 (-12.%)	4.10E-10 (-7.9%)
Case M3 PEBBED with half-step flux)	1.50E-06 (-8.4%)	1.03E-04 (-0.1%)	7.19E-07 (-4.1%)	3.35E-07 (-9.2%)	4.45E-12 (-27.%)	2.56E-11 (-12.%)	4.11E-10 (-7.5%)
Case M4 PEBBED with PEBBED flux, nominal flow rate)	1.39E-06 (-15.%)	1.03E-04 (-0.4%)	7.12E-07 (-5.0%)	3.34E-07 (-8.4%)	4.97-12 (-20.%)	2.63E-11 (10%)	3.92E-10 (-12.%)
Case M5 PEBBED with PEBBED flux, critical flow rate)	1.67E -06 (1.7%)	1.04E -04 (0.2%)	7.23E -07 (-3.5%)	3.33E -07 (-8.8%)	4.17E -12 (-33.%)	2.83E-11 (-3.3%)	3.42E-10 (-23.%)

There is no discernible trend among the results shown above between the OTTO and multipass cases. In Cases M2 and M3, there is a substantial deviation between the results compared to the OTTO case (O2b) with some exceptions, namely Gd-155. Xe-135 concentrations also show better agreement in the multipass core for the M4 and M5 cases. On the other hand, the difference in the U-235 concentration in M2 is -7.5%, whereas the OTTO case (O2b) shows very good agreement over a similar burnup range, more than what can be explained by the differences in the depletion solution methods.

The multipass cases differ from the OTTO cases of the previous section in just a few well-defined ways. The average discharge burnup of pebbles in the MEDUL core (109.9 MWD/kg of heavy metal) is higher than that of the OTTO core (97.9 MWD/kg of heavy metal) because of the better neutron economy. This can account for a small part of the differences in individual concentrations as the numerical deviation would expect to increase with burnup. The size of the individual burnup steps in the multipass cases is about $1/6^{th}$ that of the OTTO cases. In the models constructed for both VSOP and PEBBED, however, the large burnup steps in the OTTO cases were subdivided into smaller steps to prevent numerical errors. Numerical precision errors likewise are not deemed a significant contributor to the differences beyond what is observed and discussed for the OTTO case.

The main difference between the multipass and OTTO models is the fact that differences in burnup due to the nonuniform radial flux profile are cancelled after each pass. Physically and numerically this implies a more uniform burnup accrued over the full trajectory of a given pebble. Given that each batch now contains a mixture of pebbles with a wide range of burnups, the multipass calculation is likely to be more sensitive to the errors induced by the numerical

averaging procedures discussed in Section 2.3. That there is no obvious trend in the errors in going from OTTO to multipass suggests a degree of uncertainty in the mixing and averaging of nuclide concentrations that is larger than expected. Further investigation of local nuclide concentrations before and after the mixing calculations may reveal particular issues that can be resolved.

The nuclide concentrations generated by the PEBBED flux solver in the multipass cases (M4 and M5) show, on average, better agreement with VSOP than the corresponding OTTO cases, particularly with the fission products. It is possible that the mixing algorithm causes a partial cancellation of errors induced by the individual burnup solvers. A core eigenvalue of 0.9840 was computed by PEBBED using the VSOP cross sections and flow rates; a difference of about 1490 pcm from VSOP. The comparable OTTO case (O4) showed a difference of about 860 pcm. In the M5 cases, adjusting the overall pebble flow rate from 1208 pebbles per day to 1280 pebbles per day (about 6%) was enough to re-capture a critical core eigenvalue.

3. CONCLUSIONS & FOLLOW-ON ACTIVITIES

A comparison of burnup and pebble mixing algorithms used in two pebble-bed reactor fuel management codes is presented. VSOP, used for the design and analysis of the PBMR Demonstration Power Plant, uses an exponential Taylor Expansion of the transmutation matrix to solve for the actinides in its nuclide set. A finite difference solver is used to compute the concentrations of fission products. PEBBED, under development at Idaho National Laboratory, uses a sequence of linear chains solved analytically using Laplace Transforms. An independent Taylor expansion solver was used to compare the predictions of the codes for single burnup step cases.

The VSOP solver splits each burnup step into two halves, solving the first half with an initial flux vector to get the number densities at the half-step. These are used to re-compute the flux and burn the nuclides for the remaining half. PEBBED iterates between the full core burnup and flux solutions using a linear average of the substep endpoint densities to update the flux profile. Both of these approaches are approximations resulting from the discretization of the burnup profile in the core. Differences in these algorithms and averaging processes are shown to lead to differences in discharge burnup and the concentrations of individual nuclides. The concentrations are minor for the major actinides and tolerable for the direct fission products. Overall values for discharge burnup and eigenvalues are generally in agreement, but differ somewhat due to widely varying estimates of minor actinide and fission product yields.

In single burnup step studies, the VSOP matrix exponential solver yields excellent agreement with an independent matrix exponential solver. The fission product solver, on the other hand, yields erroneous results for some fission products if the duration of the burnup step is greater than about 10 days—a limitation of the finite difference solver employed. Such long steps (>10 days) are found in the analysis of OTTO fuel management schemes that are characterized by slowly moving pebble streams. To avoid significant errors in fission product buildup, the batch sizes or subdivisions in OTTO core models should be limited such that the burnup interval is <10 days.

The burnup solver in PEBBED yields reasonable results for major actinides and many fission products, but can produce significant numerical errors for minor actinides and selected fission products. These are further shown to yield significant differences in computed core power and eigenvalue. In some cases, these errors cannot be reduced simply by reducing the burnup interval, but arise from the limitations of floating point arithmetic and the widely varying transmutation rates of the nuclides in the depletion chains. The linear chain approach is also cumbersome or inadequate for low-yield interactions such as (n,2n) and alpha decay. For detailed analysis of minor actinide and fission product buildup, the solver in PEBBED should be replaced by a reliable matrix exponential solver.

A multipass (MEDUL) core was constructed with the same physical geometry, power, and fuel type. Given its similarity to the OTTO core, any differences in the results could be attributed mainly to the pebble mixing algorithms employed by the codes. The discharge isotopic concentration results were not conclusive. There was better agreement between VSOP and PEBBED for some isotopes (as compared to the OTTO cases) and less agreement between others. The overall core eigenvalue computed using the PEBBED flux solver was closer to the VSOP result in the multipass cases. This indicates that the mixing and averaging of pebbles of different burnup levels cancels some reactivity differences induced by the burnup solvers.

This study reveals the sensitivity of pebble bed equilibrium cycle calculations to differences in depletion and pebble mixing algorithms. The differences between different solvers can be significant (causing a difference in reactivity of hundreds of pcm) and results from such analyses must be reported with appropriate statements of uncertainty. Through sensitivity studies, benchmarks, and comparisons, the core analyst must also acquire a firm understanding of the limits and strengths of the algorithms embedded in the codes.

This simplified model can provide a component of a computational benchmark for a complete pebble bed reactor equilibrium cycle analysis that includes the core neutronic and thermal-hydraulic exercises specified in reference [12]. The geometry, flux, pebble flow, material, and cross section data used in this study can be obtained from the authors.

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