New Method to Analyze Equilibrium Cycle of Pebble-Bed Reactors

Hiroshi SEKIMOTO, Tohru OBARA†, Shigeru YUKINORI†† and Eiichi SUETOMI

Research Laboratory for Nuclear Reactors, Tokyo Institute of Technology*

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A new computer code PREC was developed to solve neutron and nuclide density distributions at the equilibrium cycle of pebble bed reactors. The PREC code has the following special advantages:

1. To provide a direct solution of the equilibrium cycle
2. To fix the effective multiplication factor as an input
3. To treat continuous fuel movement
4. To treat r-z two-dimensional geometry, leading in turn to the following special advantages:
   4-1. Ability to treat the cavity at the top of the core
   4-2. Ability to treat the curved fuel stream-line.

KEYWORDS: burn-up equation, computer codes, diffusion equation, distribution, effective multiplication factor, equilibrium cycle, fuel cycle, neutron flux, pebble-bed reactor, power equation, PREC, radioisotopes, SOR-Newton method, VSOP

I. INTRODUCTION

The pebble bed reactor has been developed to supply high-temperature gas to generate electricity at high efficiency and/or to provide process heat sources. Recently the superior safety features of this reactor have attracted a special interest, and a new type of the pebble bed reactor (modular high-temperature reactor) was proposed as an inherently safe reactor(1). The pebble bed reactor also has the advantage of excellent neutron economy, since it uses graphite, whose neutron capture is very small, as the construction material as well as the moderator, and need not install control rods to compensate for the excess reactivity for burnup (shim rods).

In the pebble-bed reactor, a fixed graphite reflector forms a container for the core which consists simply of a multitude of graphite balls. The balls are typically 60 mm in diameter with the required quantities of fuel particles embedded within. They are cycled slowly and continuously through the core by gravity, and can either pass through the reactor numerous times before being discarded, or only once in the so-called OTTO cycle (Once Through Then Out).

Since the refueling is continuous, after a running-in phase an equilibrium is reached, and the reactor composition does not change with time. The power profile should not be changed so much along the reactor operation, and the good profile at the beginning of the operation should be similar to the profile for the equilibrium cycle. Therefore it is important to find and investigate the equilibrium cycle. For a proper ball configuration for the initial core, the running-in period may be reduced to about 1/10 of the whole reactor operation.
life. The analysis of the equilibrium cycle gives us a good prediction of general characteristics over the entire range of reactor operation cycles.

Since the in-core fuel management for the pebble-bed reactor is entirely different from traditional nuclear reactors such as light-water reactors, the analysis of the pebble-bed reactor requires special code systems. The VSOP code system(2) may be the most popular code system to solve neutronic characteristics of the pebble-bed reactor. It simulates the fuel burnup at each real time-step from the start of the reactor operation to the equilibrium cycle, and requires extensive calculations to obtain the equilibrium cycle solution. Since the equilibrium cycle may give us a good prediction of general characteristics over the entire range of reactor operation cycles, we have developed a new code PREC (Pebble-Bed Reactor Equilibrium Cycle) to treat the equilibrium cycle directly. This code solves the neutron diffusion equation and burnup equation including ball flow simultaneously.

When some parameter (such as enrichment or moderation ratio (carbon/heavy-metal ratio) for the inserted balls) is changed to improve some burnup characteristics (maximum burnup and/or conversion ratio, for example), traditional codes such as VSOP give us the results where not only burnup characteristics but the effective multiplication factor also changes. The larger effective multiplication factor reduces the burnup characteristics and vice-versa. In that case, some other parameter must be modified to adjust this factor to the originally planned value in order to make the comparison fair. The PREC code gives us a result whose effective multiplication factor is not altered by any parameter changes by automatically adjusting the other parameters (such as moderation ratio or enrichment for the inserted balls) for a given core geometry.

It is difficult for the traditional codes to treat the continuous flow of the fuel ball through the core precisely. The VSOP code simulates the flow by approximating with discontinuous movements of fuel batches through adjacent core layers. The PREC code can treat the continuous ball flow directly.

Since the present treatment reduces the calculation time by solving the equilibrium cycle directly, we can solve the r-z two-dimensional problem without any approximations such as the separation-of-variable of flux-synthesis technique within a reasonable calculation time. The precise two-dimensional treatment makes possible to treat the cavity at the top of the core and the curved ball flow along the funnel-shaped side wall of the core in good accuracy.

The equations describing the neutron transport and fuel burnup are presented in Chap. II, and the method to solve these equations is shown in Chap. III. Some computational results and summary are given in Chaps. IV and V, respectively.

II. EQUATIONS

1. Diffusion Equation

The neutron transport is treated with the following r-z two-dimensional multi-group diffusion equation:

\[
\frac{1}{r} \frac{\partial}{\partial r} r D_g \frac{\partial}{\partial r} \phi_g + \frac{\partial}{\partial z} D_g \frac{\partial}{\partial z} \phi_g - \sum_{i} \sigma_{i, r, g} N_i \phi_g + \sum_{j} \sigma_{i, g-1, j} N_j \phi_{g-1}
\]

\[
+ \frac{\chi_g}{k_{\text{eff}}} \sum_{g'} \sum_{i} \nu \sigma_{i, f, g'} N_i \phi_{g'} = 0, \tag{1}
\]

where

- \( \phi_g \) : Neutron flux in energy group \( g \)
- \( N_i \) : Atomic density of isotope \( i \)
- \( D_g \) : Diffusion coefficient for group \( g \)
- \( \sigma_{i, r, g} \) : Removal cross-section of isotope \( i \) for group \( g \)
- \( \sigma_{i, g-1, j} \) : Slowing-down cross-section of isotope \( i \) from group \( g-1 \) to \( g \)
- \( \sigma_{i, f, g} \) : Fission cross section of isotope \( i \) for group \( g \)
- \( \nu \) : Average number of fission neutrons released in fission reaction
- \( \chi_g \) : Probability that fission neutron will be born with energy in group \( g \)
- \( k_{\text{eff}} \) : Planned effective multiplication factor.

The summation for index \( i = HN \) extends to all heavy nuclides. The effective multiplication factor \( k_{\text{eff}} \) in Eq. (1) is not an eigenvalue but a planned value, and some other parameter (such as enrichment or moderation ratio for the inserted balls) is adjusted to hold Eq. (1).
The group constants and their changes with respect to temperature $T$ and atomic density of influential nuclide $\rho$ have been calculated using a part of VSOP code system (THERMOS, GAM etc.). In the PREC code the changes of the constants for important nuclides $^{232}$Th, $^{233}$U, $^{233}$Pa, $^{234}$U, $^{135}$Xe, $^{149}$Sm are evaluated by using the shielding factor calculated with the following equation:

$$S = 1 + a_1 \Delta T + a_2 \Delta \rho + a_3 T^2$$

$$+ a_4 T \Delta \rho + a_5 \Delta \rho^3,$$  \hspace{1cm} (2)

where the coefficients $a_i$ have been determined from least-square fitting for many spectral calculation results obtained with VSOP.

2. Burnup Equation

The nuclides contained in the ball move through the core, and the number density for each nuclide satisfies the following materials balance equation:

$$- \frac{dN_i}{ds} = \sum \lambda_i \alpha_{i'-i} N_{i'}$$

$$+ \sum_g (\sigma_{i', g} + \Sigma_a N_{i'} \phi_g)$$

$$+ \sum_g \sigma_{i', f, g} \gamma_{i'-i, g} N_{i'} \phi_g$$

$$- \lambda_i N_i + \sum_g (\sigma_{i, a, g} N_i \phi_g) = 0,$$  \hspace{1cm} (3)

where

- $s$: Distance measured along ball stream line
- $\gamma_i$ and $\gamma_X$ are the effective fission yields of $^{135}$I and $^{135}$Xe, respectively, and $\lambda_X$ is the $\beta$-decay constant for $^{135}$Xe.

3. Power Equation

The total power output $P$ of the reactor may be written with close accuracy as

$$P = CF,$$  \hspace{1cm} (5)

where $C$ is the energy released per fission, and $F$ the total number of fissions in the core, which can be written as

$$F = \int_{\text{core}} \left( \sum_{i' \in N} \sigma_{i, f, g} \phi_g \right) dV.$$  \hspace{1cm} (6)

This quantity can be written also as

$$F = \sum_{k} \sum_{i' \in N} V_s [N_{i, k} (\text{charge})$$

$$- N_{i, k} (\text{discharge})],$$  \hspace{1cm} (7)

where the suffix $k$ denotes the ball moving pattern through the core, and $V_s$ is the volume of the inserted (or discharged) fuel per unit time for pattern $k$.

Although Eqs. (6) and (7) should coincide with one another, there may be differences caused by the numerical calculation errors such as round-off and discretization errors. This difference can be used as a performance index of the accuracy of calculation.

### Table 1: Nuclides employed in code

<table>
<thead>
<tr>
<th>Heavy nuclides</th>
<th>$^{233}$Th, $^{233}$Pa, $^{235}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{239}$Np, $^{239}$Pu, $^{241}$Pu, $^{242}$Pu, $^{244}$Pu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fission products</td>
<td>$^{55}$Fe, $^{60}$Zn, $^{65}$Mo, $^{69}$Tc, $^{93}$Ru, $^{95}$Ru, $^{140}$Rh, $^{140}$Rh, $^{140}$Nd, $^{140}$Nd, $^{140}$Nd, $^{142}$Sm, $^{146}$Sm, $^{146}$Sm, $^{147}$Sm, $^{147}$Sm, $^{147}$Sm, $^{150}$Sm, $^{151}$Sm, $^{153}$Sm, $^{154}$Eu, $^{154}$Eu, $^{156}$Eu, $^{156}$Gd, $^{156}$Gd, $^{156}$Gd, $^{157}$Gd, Non-saturating FP</td>
</tr>
<tr>
<td>Scatters</td>
<td>$^{12}$C, $^{16}$O</td>
</tr>
<tr>
<td>Poison</td>
<td>$^{68}$Po, Impurity in C</td>
</tr>
</tbody>
</table>

where $\gamma_i$ and $\gamma_X$ are the effective fission yields of $^{135}$I and $^{135}$Xe, respectively, and $\lambda_X$ is the $\beta$-decay constant for $^{135}$Xe.
III. NUMERICAL ANALYSIS

1. Discretization

By using the finite difference approximation for space variable, Eq. (1) is transformed to the following system of algebraic equations:

\[ f_{g,m} (\cdots, \phi_{g,m}, \cdots, N_{i,m}, \cdots, x) = 0, \quad (8) \]

where \( x \) is the characteristic value of the enrichment or moderation ratio for the inserted balls, and the suffix \( m \) denotes the \( m \)-th spatial mesh point.

By the same way, Eq. (3) is also transformed to the following system of equations:

\[ g_{i,m'} (\cdots, \phi_{g,m'}, \cdots, N_{i,m'}, \cdots, x) = 0. \quad (9) \]

The mesh points \( m' \) are on the stream lines. The nuclide number density is determined in turn from the density at the upper mesh point on the same stream line. The mesh widths are changed for different nuclides. They are chosen to be smaller for the nuclides whose changes along burnup are rapid and important.

The mesh point \( m' \) for Eq. (9) does not coincide with \( m \) for Eq. (8) in general. By utilizing the interpolation for the radial axis, the neutron flux at \( m' \) is evaluated from the fluxes at \( m \) obtained by Eq. (8) and used to calculate the nuclide density in Eq. (9). In the same manner, the nuclide density at \( m \) is evaluated from the densities at \( m' \) obtained by Eq. (9) and used to calculate the neutron flux in Eq. (8).

Equation (6) or (7) is also transformed to

\[ h(\cdots, \phi_{g,m'}, \cdots, N_{i,m'}, \cdots, x) = 0, \quad (10) \]

where mesh point \( m'' \) coincides with \( m \) for Eq. (10) derived from Eq. (6), and with \( m' \) for Eq. (10) from Eq. (7).

2. SOR-Newton Method

The obtained system of equations are nonlinear, and solved by SOR-Newton method to obtain \( \phi_{g,m} \) and \( N_{i,m} \) simultaneously, for which the iteration scheme is given as follows:

\[ \phi^{(l)}_{g,m} = \phi^{(l-1)}_{g,m} - \omega_{N} \frac{f_{g,m}}{\partial \phi_{g,m}} \]

\[ N^{(l)}_{i,m} = N^{(l-1)}_{i,m} - \omega_{N} \frac{g_{i,m'}}{\partial N_{i,m'}} \]

\[ x^{(l)} = x^{(l-1)} - \omega_{x} \frac{h}{\partial x} \]

for the \( l \)-th iteration, where \( \omega_{N} \), \( \omega_{x} \), and \( \omega_{x} \) are relaxation parameters, and usually \( \omega_{N} = 1 \).

The direction for solving Eq. (12) is chosen to be the ball flow direction. For \( \omega_{N} = 1 \), \( N^{(l)}_{i,m} \) can be calculated without using \( N^{(l-1)}_{i,m} \). The values for \( l = 0 \), \( \phi^{(0)}_{g,m}, N^{(0)}_{i,m}, \) and \( x^{(0)} \), are given as initial guesses.

3. Calculation Flow

The flow of the calculation is shown in Fig. 1. Before the iteration starts, the standard microscopic cross section set and the shielding factor coefficient set are prepared by the cell calculations with a separated code.

The calculated results are generally stored in files, and used as initial guesses for future calculations. When these values are not available, flat guesses are used. For \( \omega_{N} = 1 \), nuclide density guesses are used only for calculating the neutron flux at \( l = 1 \), since \( N^{(1)}_{i,m} \) can be calculated without using \( N^{(0)}_{i,m} \).

The flux \( \phi^{(1)}_{g,m} \) is affected directly by \( \phi^{(l-1)}_{g,m} \). Inner iterations for the flux are performed for \( l = 1 \) and 2, where the shape of \( \phi^{(1)}_{g,m} \) is far from the solution. The convergence criterion for the inner iteration is much larger than the final criterion, and usually set to be 0.1.

The iterative calculation is considered to be converged, when the following criteria are satisfied:

\[ e^{(l)}_{\phi} = \frac{\sqrt{\sum_{m} \sum_{g} \left( \phi^{(l)}_{g,m} - \phi^{(l-1)}_{g,m} \right) \Delta V_{m}}}{\sum_{m} \sum_{g} \phi^{(1)}_{g,m} \Delta V_{m}} \leq \varepsilon_{\phi}, \]

where \( \Delta V_{m} \) is the volume element of the mesh \( m \).

\[ e^{(l)}_{\phi} = \frac{\max_{m} \left| \phi^{(l)}_{g,m} - \phi^{(l-1)}_{g,m} \right|}{\max_{m} \phi^{(1)}_{g,m}} \leq \varepsilon_{\phi}, \]

\[ e^{(l)}_{\phi} = \frac{\max_{m} \left| N^{(l)}_{i,m} - N^{(l-1)}_{i,m} \right|}{\max_{m} N^{(1)}_{i,m}} \leq \varepsilon_{\phi}, \]
where the convergence of $N_{i,m'}^{(l)}$ is checked only for important nuclides. The following further criterion is used for total power, average burn-up for discharged fuels, conversion ratio and moderation ratio (or enrichment) for the inserted balls,

$$e_y^{(l)} = \frac{|y^{(l)} - y^{(l-1)}|}{y^{(l)}} \leq \varepsilon_y.$$  

**IV. SAMPLE PROBLEM**

1. **Verification**

The calculation has been performed for a
different number of mesh points. The number of mesh points was increased until the calculated results gave the same answer.

The accuracy of two-dimensional diffusion calculation was verified by comparing the PREC results with the results calculated with the CITATION code\(^4\) using the macroscopic cross sections obtained from the PREC calculation. Though the macroscopic cross section is given for each diffusion calculation mesh in the PREC code, the same value was given for each mesh point in the same cross section zone for the CITATION calculation. The difference of the neutron flux between these two calculations

\[
\delta \phi = \frac{\sqrt{\sum m (\phi_{m}^p - \phi_{m}^c) dV_m}^2}{\sum m \phi_{m}^p dV_m},
\]

was generally about 0.2% for each group. The difference of the effective multiplication factor was about 0.4%. These values seem to be small enough considering several differences of the calculational conditions.

The accuracy of the burnup calculation was checked by comparing with the VSOP calculations. The difference of the average burnup of the discharged fuel was generally about 1%. This amount of error seems to be reasonable, since the VSOP code performs the burnup calculation by using the fuel layer, which may cause some error.

The difference of the total power calculated with Eqs. (6) and (7) was generally about 2%. This may be attributed to the difference of the contributing mesh points for both calculations.

2. Demonstration

A calculated result for the THTR reactor is shown as an example. The nuclides employed in the code and the neutron energy group structure are given in Table 1 and Table 2, respectively.

Since the PREC code treats r-z two-dimensional geometry, the cavity at the top of the core was dealt with using the method developed by Gerwin \& Scherer\(^5\), where the reaction

![Fig. 2 Calculation geometry](image)

<table>
<thead>
<tr>
<th>Table 2 Neutron energy group structure for standard calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Group</strong></td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3 Calculation conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Thermal power</strong></td>
</tr>
<tr>
<td><strong>(k_{\text{eff}})</strong></td>
</tr>
<tr>
<td><strong>Top reflector</strong></td>
</tr>
<tr>
<td>Atomic density of C</td>
</tr>
<tr>
<td><strong>Side and bottom reflector</strong></td>
</tr>
<tr>
<td>Atomic density of C</td>
</tr>
<tr>
<td><strong>Upper cavity diffusion coefficients</strong></td>
</tr>
<tr>
<td>(D_i)</td>
</tr>
<tr>
<td>(D_t)</td>
</tr>
<tr>
<td><strong>Fuel velocity at center top of core</strong></td>
</tr>
<tr>
<td>1.35 \times 10^{-4} \text{ cm/s}</td>
</tr>
<tr>
<td><strong>Av. residence time of fuel</strong></td>
</tr>
<tr>
<td><strong>Fuel element</strong></td>
</tr>
<tr>
<td>Ball diameter</td>
</tr>
<tr>
<td>Thickness of graphite shell</td>
</tr>
<tr>
<td>Graphite density</td>
</tr>
<tr>
<td><strong>Coated particle</strong></td>
</tr>
<tr>
<td>Kernel</td>
</tr>
<tr>
<td>Material</td>
</tr>
<tr>
<td>Diameter</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Coating (from inner)</td>
</tr>
<tr>
<td>Material</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Thickness</td>
</tr>
<tr>
<td><strong>Fuel cycle</strong></td>
</tr>
</tbody>
</table>
Fig. 3 Neutron flux distribution
cross sections in the cavity were zero, and the diffusion coefficients were treated to be large and different in their radial and axial directions. The stream lines of the fuel balls employed in the present calculation were evaluated from the intensive studies by Bedenig et al.\(^6\) The calculation geometry is shown in Fig. 2, where the ball stream lines and the ball velocity distribution at the top of the core are also shown. Other calculation conditions are given in Table 3.

The obtained neutron flux distribution is shown in Fig. 3, and other results are given in Table 4. Two figures of flux different for the view directions are presented for each energy group to facilitate viewing the effects of cavity and bottom shape. The flux shapes are similar for 1st~3rd groups, and the neutrons flow into the cavity from the core and out to the reflector. The 4th group flux shows the complicated structure caused by the neutron stream from the reflector to the cavity.

**Table 4 Calculated results**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal power</td>
<td>698 MW</td>
</tr>
<tr>
<td>Av. burnup of discharged fuel</td>
<td>79,071 MWD/t-HM</td>
</tr>
<tr>
<td>Conversion ratio</td>
<td>0.564</td>
</tr>
<tr>
<td>Moderation ratio of loaded fuel</td>
<td>500</td>
</tr>
</tbody>
</table>

The required calculation time is smaller than the VSOP calculation for the similar problem.

**V. SUMMARY**

The new code PREC was developed to solve the equilibrium cycle of the pebble bed reactor directly as a nonlinear problem associated with the neutron flux, nuclide densities and total power. The accuracy of the code was verified by investigating the effects of the mesh spacing and by comparing with the calculations by the other codes, CITATION and VSOP.

The PREC code has the following characteristics:

1. Direct solution of the equilibrium cycle
2. To fix the effective multiplication factor as an input (desirable characteristic for parametric surveys)
3. Ability to treat the continuous ball flow
4. To treat \( r-z \) two-dimensional geometry
   4.1 Ability to treat the cavity at the top of the core
   4.2 Ability to treat the curves of the ball flow.

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