HTR-10 OTTO Cycle Depletion Simulation Using Discrete Element Method Coupled Monte Carlo

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Abstract. Pebble bed reactor core contains 27,000 pebbles placed in a random position. Since the pebble insertion relies on gravity, the pebble placement pattern is irregular. Discrete Element Method used to simulate the pebble interaction and pebble movement during HTR-10 operation. Even though pebbles distributed randomly, the random generation of pebble positions used in most research does not mimic the actual pebble position and pebble surface contact. The Discrete Element Method provides a realistic interpretation of the pebble position by considering the pebble surface contact and gravity force. Each pebble coordinates from the Discrete Element Method obtained to construct Monte Carlo geometry of the HTR-10 core realistically. By coupling the DEM simulation with Monte Carlo simulation, it is possible to calculate the depletion while considering the core dynamic characteristic. The OTTO recirculation depletion calculation scheme with steady 10MW power for 368 days was constructed and demonstrated in this work. The DEM coupled Monte Carlo method allow one to track and predict each depleted fuel composition. Although the flux distribution change is slight in every timestep, the relation between flux and depleted U$^{235}$ and Xe$^{135}$ composition deserves to be taken into account. The calculation model in this work is comparable with the other calculation, but the timestep adjustment is needed to provide more accurate and representative results. Flux calculation and depletion simulation performed using the OpenMC program with ENDF/B-VIII.0 cross-section data. Please refer to digital version to view graph.

1. Introduction
Nuclear energy is a viable option for high power baseload generation with zero carbon emission. The development of a safer and more financially competitive reactor design could stimulate the nuclear power generation industry growth for the future. For many decades to come, the Generation IV reactor will be dominating the nuclear energy market with modular reactor design and advanced operation technology aiming to answer safety and financial challenges. One of the Generation IV reactors with mature technology for power generation is High-Temperature Reactor (HTR).

HTR is a type of reactor that operates at a higher temperature than the conventional light water reactor. The most interesting HTR design is the Pebble Bed Reactor (PBR). PBR uses a discrete spherical Tristructural-Isotropic fuel element (TRISO) coated in the graphite matrix to form a spherical-shaped fuel. The reactor core was constructed with stacked graphite blocks with a cavity to contain the pebble. Due to its fuel shape, the reactor able to perform online refueling or a fuel recirculation scheme. The PBR core cooled with gases such as helium or carbon dioxide. One of the PBR is HTR-10 in which was constructed by the Institute of Nuclear Energy Technology (INET) at Tsinghua University[1].

The core of PBR fills with randomly arranged spherical fuel pebbles. The absence of a fuel placement pattern caused the neutronic simulation geometric definition hard to construct. There is two randomness...
considered in modelling the PBR geometry for reactor simulation or neutronic calculation. The randomness includes random placement of the TRISO element inside the fuel pebble matrix also random arrangement of the pebble inside the core. Most of the HTR-10 benchmark models employ the lattice pattern to define the double randomness of the reactor. The lattice model creates uniform packing density and less pebble-to-pebble surface contact.

In a time-dependent problem such as a calculation of depleted material, the geometrical modelling of the core needs to consider the change of pebble position every timestep. The reactor can perform online refueling by recirculating the pebble in the reactor core due to the spherical-shape fuel pebble and hopper shaped core vessel. That means, the geometric model for each simulation period needs to be updated with a different set of pebble position according to its move during that period to represent the pebble movement. Therefore, the calculation needs an infinite number of models to solve a certain length of the time-dependent problem.

Only fresh fuels are allowed to enter the reactor core in the Once-Through Then-Out recirculation scheme. The previous research employs a layer-to-layer method to model the pebble recirculation [2]. Layer-to-layer method group the pebbles with the coolant in an axial or a radial region as a cell. After a certain timestep of depletion calculation, the material of a specific cell changed with depleted material of the cell located above the specified cell for the next depletion calculation [2]. However, that method neglects three-dimensional pebble displacement and the double randomness in the PBR core.

This study will create an HTR-10 model to simulate and calculate the flux tally problem by considering its time-dependent behavior. The study demonstrated a new approach to make a very high-fidelity Monte Carlo geometry model and simulation sequence for time-dependent problems.

2. Model construction

2.1. HTR-10 Core Geometry

The reactor model is similar to the benchmark models provided by IAEA TecDoc [1]. The detailed description of material composition data obtained from the IRPhEP report [3] which based on the IAEA technical document. There are 83 zones of reactor geometry with different compositions of carbon, boron, and coolant. Some region such as Fuel region, reflector boring, and control channel modelled resembling the description in the high-fidelity benchmark model in [1], [3]. There are 28,020 pebbles with 24,531 mixture pebbles inside the core zone at initial (t=0).

Each pebble modelled as a 3 cm radius sphere with center coordinate obtained from DEM simulation. The bottom part of the discharge tube modelled as a homogenous cell represents dummy pebbles similar to the benchmark model from IRPhEP [3]. The bottom surface of the core descends by following the lower position of the simulated pebble step. Each fuel pebble contains an exact 8,335 TRISO scattered randomly inside fuel zone. Each TRISO center point has a distance between one another same or above 1 mm.

| Table 1. TRISO Material Properties |
|-----------------------------------|
| Matrix Density                  | 1.73 g/cm³   |
| Uranium Mass/Pebble             | 5 g          |
| Uranium Enrichment              | 17 wt.%      |
| Boron content in Kernel         | 4 ppm        |
| TRISO Layer                     | Kernel/Buffer/PyC/SiC/PyC |
| Layer Thickness (mm)            | Ø=0.5/0.04/0.035/0.04/0.09 |
| Density (g/cm³)                 | 10.4/1.1/1.9/3.18/1.9 |
Figure 1. OpenMC HTR-10 model cross-section view z=0 and TRISO detail.

Figure 2. OpenMC HTR-10 model cross-section view x=0 at depletion step 0.

2.2. DEM Simulation
DEM simulation is used to map the center point of each pebble inside the core. Simulation performed by LAMMPS Improved for General Granular and Granular Heat Transfer Simulations (LIGGGHTS) open-source DEM code [4]. DEM simulation tracks each particle to simulate the particle contact and force balance of the particle. The force related parameter such as young modulus, friction coefficient, and Poisson ratio fed to DEM simulation. Particle to particle contact model used a linear spring and dashpot model with normal force and tangential force written as[4]:

\[
\text{ force } = \begin{cases} 
K & \text{if } |\text{displacement}| < \text{critical distance} \\
K\text{critical distance} & \text{if } |\text{displacement}| \geq \text{critical distance} 
\end{cases}
\]
\[ F_n = -k_n \delta_n + c_n \Delta u_n \]  
\[ F_t = \min \left\{ \left[ \int_0^t \Delta u_t \, dt + c_t \Delta u_t \right] \mu F_n \right\} \]  

Where \( F_n \) is the normal force, \( F_t \) is the tangential force, \( k_n \) and \( k_t \) are spring coefficient for normal or tangential force, \( c_n \) and \( c_t \) are damping coefficient for normal or tangential force, \( u_n \) and \( u_t \) are velocity component, \( \delta_n \) is normal overlap between particle, and \( \mu \) is friction coefficient. From this equation, the simulation allows overlap between particles, especially for soft particles. For solid granular such as PBR pebble in this study, the overlap created as low as possible (\( \delta_n = 0.01 \text{ mm} \)).

The inner core boundary modelled in STL surface mesh format. Since the user did not allow the pebble to free fall from the core boundary, the discharge tube shuts with a movable plane called "stopper" to control slow discharge. For the initial configuration, the stopper placed at -143.182 cm level.

| Table 2. Physical properties of pebble particle for DEM simulation. |
|---------------------------------------------------------------|
| Parameter                  | Value             |
|---------------------------|-------------------|
| Radius                    | 3 cm              |
| Density (Fuel/Dummy)      | 1.857; 1.790 g/cm³|
| Young’s Modulus [5]       | \( 10^9 \text{ Pa} \) |
| Friction Coefficient [5]  | 0.7               |
| Poisson Ratio [5]         | 0.3               |
| Timesteps                 | 50 \( \mu s \)    |

2.3. Monte Carlo Simulation

Monte Carlo simulation in this study used OpenMC open-source code [6]. OpenMC code provided python Application Programming Interface (API) to ease the modelling and tally data processing. The API will automate the whole simulation methodology in this research. The simulation in this work used Evaluated Nuclear Data File (ENDF) version B-VIII.0 neutron cross-section library with ACE file format preprocessed with NJOY21 [7]. OpenMC reads HDF5 cross-section data converted from ACE file to perform the calculation [8]. This work used PWR-simplified chain for the VERA benchmark suite that includes 255 nuclides for depletion simulation [9].

Monte Carlo simulation in this work will simulate initial criticality case and full core case with various ENDF library to validate the model and compare the \( k_{\text{eff}} \). Those simulations used 10,000 particles per cycle with 500 active cycles and 50 inactive cycles (5,000,000 neutron histories). Besides, Monte Carlo depletion simulation simulated 5,000 particles per cycle with 200 active cycles and 10 inactive cycles (1,000,000 neutron histories). The depletion will perform 368 days operation with 17 unequal length timestep. The integrator used for depletion simulation is high order EPC-RK4. EPC-RK4 was used due to its low relative error to exponential matrix method and low standard deviation than the Predictor-Corrector method, Exponential Linear, and CE/CM (constant extrapolation on predictor and constant midpoint on Corrector) performed by the previous research [10]. In exchange, the EPC-RK4 will simulate Monte Carlo transport four times in a timestep to solve functions order of its algorithm.
3. Calculation Algorithm

![Diagram](image)

*Figure 3. DEM coupled Monte Carlo method depletion simulation flowchart.*

The pebble enters the reactor one by one from the 10cm diameter aperture above the reactor boundary. The total DEM timestep from the insertion of dummy pebble until all 28,020 pebbles settled ($E_k \leq 10^{-5}$ J) is 8,600,000 timestep. The stopper went down 1 cm/day of depletion timestep length to...
represent core height descend. Let \( D \) is a depletion time in days, then the timesteps to simulate the stopper go down is \( 5,000D \). After that, the set of unirradiated pebble inserted for the next \( 5,000D \) to compensate for the core height descend. DEM will also simulate 100,000 timesteps to make sure the pebbles are all settled. Therefore, the total timesteps performed from one depletion step to another is \( 10,000D + 100,000 \) timesteps. The relation of DEM timesteps and Monte Carlo depletion steps shown in Figure 4.

![Figure 5. Fuel pebble grouping rule at initial depletion step.](image)

Ideally, to perform the depletion for OTTO recirculation, each fuel pebble must be tracked individually to give an exact number of fissile materials depleted inside each fuel pebble. For simplification, the fuel pebble grouped according to its center cylindrical coordinates at timestep 0. In the initial configuration (step 0), there is 15 fuel pebble group. The fuel pebble grouping rule showed on Figure 5. Each fuel pebble in a pebble grouping has the same kernel material properties and tracked every Monte Carlo calculation step. In every step, the depletion of each pebble group accounted for the next Monte Carlo step. The newly added fuel has three groups specified by its center radial coordinate. In total, there are 66 fuel groups for 17 depletion steps (\( 15 + 3 \times \text{[step]} \)).

| Fuel Pebble | Total Pebble in DEM | Total Pebble in MC core | Day | Depletion Step | Active height [cm] |
|-------------|---------------------|-------------------------|-----|----------------|-------------------|
| 13981       | 28020               | 28020                   | 0   | 0              | 208.12            |
| 14006       | 28064               | 28064                   | 7   | 1              | 210.97            |
| 14029       | 28106               | 28106                   | 14  | 2              | 211.544           |
| 14052       | 28148               | 28148                   | 21  | 3              | 212.172           |
| 14073       | 28186               | 28186                   | 28  | 4              | 213.213           |
| 14100       | 28235               | 28235                   | 38  | 5              | 214.161           |
| 14127       | 28284               | 28284                   | 48  | 6              | 213.627           |
| 14153       | 28331               | 28331                   | 58  | 7              | 212.981           |
| 14180       | 28379               | 28379                   | 68  | 8              | 214.728           |
| 14305       | 28599               | 28599                   | 98  | 9              | 213.998           |
| 14431       | 28821               | 28694                   | 128 | 10             | 213.513           |
| 14559       | 29047               | 28659                   | 158 | 11             | 214.316           |
| 14682       | 29264               | 28618                   | 188 | 12             | 213.596           |
| 14810       | 29490               | 28570                   | 218 | 13             | 210.829           |
| 14933       | 29706               | 28521                   | 248 | 14             | 213.719           |
| 15048       | 29935               | 28488                   | 278 | 15             | 212.615           |
| 15132       | 30161               | 28438                   | 308 | 16             | 211.405           |
| 15192       | 30391               | 28396                   | 338 | 17             | 210.875           |
The programs run on a personal computer with 16 GB of memory and 16 threaded CPU with a 3.7 GHz maximum clock speed for each CPU core.

4. Result

4.1. Multiplication Factor

The neutron data in this calculation used room temperature at approximately 20°C. The multiplication factor from step 0 depletion and initial criticality shows that they were comparable with the other code. The initial criticality model used a similar modelling principle with the full core model. Instead of using 24,531 mixed pebbles, the initial criticality used 16,890 mixed Pebbles above level 0 cm. It appears that the model criticalities are sensitive to neutron cross-section library. Other than that, the packing of pebble inside the core gave a significant difference in reactor criticality. The full core model in this work has a maximum core height of 208.12 cm different from its closer counterpart, from [11], in which has lower core height at the full core. Therefore, this work’s full core model is less packed than another model, even though the criticality is close.

Table 4. $K_{eff}$ comparison between different code and neutron cross-section library for initial criticality and full core case.

| Calculation                  | Criticality          | Library          |
|------------------------------|----------------------|------------------|
| **Initial Criticality**      |                      |                  |
| This Work                    | $1.01762 \pm 4.1 \times 10^{-4}$ | ENDF B-VII.0    |
|                              | $1.00692 \pm 4.3 \times 10^{-4}$ | ENDF B-VII.1    |
|                              | $1.00924 \pm 4.2 \times 10^{-4}$ | ENDF B-VIII.0   |
| IRPhEP [3] (MCNP)            | $1.01190 \pm 2.1 \times 10^{-4}$ | ENDF B-VI       |
| Ref. [12] (MCNP)             | $1.00366 \pm 4.1 \times 10^{-4}$ | ENDF B-VII.0    |
| INL [11] (Serpent)           | $1.01025 \pm 5.1 \times 10^{-5}$ | ENDF B-VI       |
|                              | $1.00023 \pm 2.3 \times 10^{-5}$ | ENDF B-VII.1    |
| **Full Core**                |                      |                  |
| This Work                    | $1.14467 \pm 4.0 \times 10^{-4}$ | ENDF B-VII.0    |
|                              | $1.13298 \pm 4.1 \times 10^{-4}$ | ENDF B-VII.1    |
|                              | $1.13403 \pm 4.4 \times 10^{-4}$ | ENDF B-VIII.0   |
| INL [11] (Serpent)           | $1.12242 \pm 1.3 \times 10^{-4}$ | ENDF B-VII.1 26,992 Pebble |
| Iran [12] (MCNP)             | $1.14545$            | ENDF B-VII.0 24,705 Pebble |
| France [1]                   | $1.14737$            | VSOP             |
| China [1]                    | $1.1358$             | VSOP             |
|                              | $1.1381$             | MCNP4A           |
| Turkey [1]                   | $1.0941$             | ENDF B-IV        |
|                              | $1.0809$             | ENDF B-V         |
| USA [1]                      | $1.1298$             | ENDF B-VI        |

The $k_{eff}$ results for a different time show that the value decreased drastically only in the first step (7 days). For the rest of the time, the $k_{eff}$ decreases almost linearly. The spike or $k_{eff}$ jump happens during the addition of pebble. The $k_{eff}$ jump is barely recognizable after 38 days because fuel and dummy pebble distributed evenly in the reactor. If the simulation timestep period decreased along with lower addition each time step, the calculation should be much smoother and shows a perfect $k_{eff}$ curve without the spike.
The spectrum tally shows an ordinary thermal reactor spectrum with spikes at the thermal energy. Those means that the code and the library work properly to differentiate the neutron energy. However, Figure 7 does not show the multiple group cross-section used in transport simulation since this study utilizes the continuous neutron spectrum for transport simulation.

**Figure 6.** Combined $k_{\text{eff}}$ vs time in days.

**Figure 7.** Neutron Spectrum tally with 50 log spaced energy.
4.2. Tally Distribution

Figure 8. Pebble distribution and radial-axial flux distribution (A) after 338 days and (B) at initial, Axial flux distribution (C) after 338 days and (D) at initial, and Radial distribution (E) after 338 days and (F) at initial.

Tally calculation in this study utilizes the functional expansion of OpenMC, mesh tally and cell tally to score flux tally. The tally scoring used the 10th order Legendre Polynomial for axial distribution and 10th order Zernike Radial Polynomial for radial distribution. The score was divided into four energy spectra. Other than that, the mesh tally with $3 \times 3 \times 3 \, \text{cm}^3$ size mesh was used to filter flux tally in the reactor. The cell tally also scores the flux tally for every fuel pebble.

The graph from each cylindrical dimension (Figure 8) shows a slight oscillation because of the polynomial function behavior. The distribution shows that most of the neutron is a thermal neutron and neutron between $1\,\text{eV}$ and $1\,\text{MeV}$ spectra. Because of the longer energy gap in filter $1\,\text{eV}$ to $1\,\text{MeV}$, those energy ranges have tally distribution almost the same as thermal energy distribution. In step 0, the $1\,\text{eV}$ to $1\,\text{MeV}$ neutron spectra has a higher peak in axial distribution than the thermal neutron range.

The deviation for the tally is too small to plot and becomes unrecognized in the plot. The tally distribution concludes that the flux distribution is barely changing during recirculation. Flux normalization to units of $\frac{n}{\text{cm}^2\text{s}}$ is necessary for further analysis.

The combination of axial-radial distribution and fuel pebble distribution shows the fuel pebble in one group may receive different flux. In detail, the fuel pebble flux visualized on Figure 10. Every color on Figure 8 (A) and (B) represent different fuel pebble group but the recirculated fuel pebble is barely visible due to its small amount. At day 338, several group-1 pebbles (center and lower group) began to
exit the reactor. The fuel pebble on the discharge tube is barely perform fission due to the low flux received.

4.3. Depletion
The main feature of this method is the one could know the composition of each pebble or each group pebble. This method is useful for safeguard purposes to track and predict fuel pebble composition along with the operation. With the depletion analysis, the cause of flux fluctuation could be determined.

Some absorber Build-up such as Xe$^{135}$ caused the steep decrease in criticality at early operation. However, those Xe$^{135}$ jump from newly added fuel is insignificant due to the low amount of fuel pebble added. The relation between the residence time and Xe$^{135}$ densities shows that the recirculated pebbles deplete in a particular pattern. The trendline from Xe$^{135}$ composition of newly added fuel to residence time fit with an exponential curve that almost linear. The Xe$^{135}$ on a group-1 fuel pebble steeply decrease after 158 days due to lesser flux received by those fuel pebble in discharge tube. In the end, the Xe$^{135}$ concentration became steady after those pebbles exits the core.

![Graph](image)

**Figure 9.** U$^{235}$ and Xe$^{135}$ atom density in fuel pebble vs residence time.

The same phenomenon also happens with U$^{235}$ nuclide. The center group deplete faster than the outer radial group due to concentrated flux at the core center. Different from Xe$^{135}$ profile, the U$^{235}$ composition to residence time profile for the initial loading fuel pebbles widen. At day 248, the U$^{235}$ composition in group-1 fuel pebble begins to steady until it exits the core. Similar to Xe$^{135}$, the U$^{235}$ composition of newly added fuel creates an exponential trendline.
5. Conclusion

The method of coupling DEM with Monte Carlo simulation could create realistic geometry of HTR10. With the methodology provided in this work, one could investigate each pebble composition by grouping them and tracking its movement along with the operation. The result of this calculation is comparable with a similar modelling method or other older modelling method. However, this calculation method needs more sensitivity analysis on DEM parameter to create a comparable model with the other benchmark. It is also necessary to perform a longer depletion simulation to give a more representative relation between fuel pebble residence time and nuclide composition.

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