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Monte-Carlo Techniques to Simulate Pebble Dislocations in a PB-MR during Depletion

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The study presented in this paper has been carried out in the framework of collaboration among University of Rome and Italian National Agency for New Technologies, Energy and Environment (ENEA). It was aimed at identifying and developing a simplified, suitable method to simulate the pebble depletion in a PB-MR [Pebble-Bed Modular Reactor] for design purposes. The method is based on Monte Carlo simulation of the pebble movements within the core according to a given geometry configuration.

KEYWORDS: **PB-MR**, **pebble bed, Monte Carlo, burn-up, transition matrix**.

1. Introduction

PB-MR [**1-2**] is made of a bulk of small pebbles having, each, an independent history during its downward motion within the core and, as consequence, achieving, at each instant of the reactor life, a different burn-up. The pebble burn-up distribution within the PB-MR has an immediate, measurable impact on reactivity, core stability and cycle performance. Thus, it is worth accounting for it in a simplified, but effective way when performing process studies of such cores. The methodology described here is aimed at simulating the depletion of the pebbles during their cyclical motion in the core. The PB-MR core geometry has been described in a simplified geometry, as a finite orthogonal cylinder followed at the bottom by a truncated cone turned upside down (see Fig.1). At each fixed time interval, the pebbles make an average downward step, consequent to the drop of a pebble at bottom. This (average) step is obviously constant in the cylindrical region, while it gradually increases as the pebbles proceed toward lower positions. To represent this stepwise process, we assume a fixed discrete geometry consisting of spheres (of the pebble size) spatially distributed following given compaction laws. Each sphere position is indexed, as well as, independently, each pebble. As pebble discharge at bottom, vacancies move random from bottom and annihilate at the top, with the re-entering on top of the core of the dropped particle, or a fresh one, depending whether the dropped one has reached, or not, a prefixed burn-up limit. The random pathways follow probability laws taking into account the constraints and gravity forces. The pebbles in the core are subdivided, accordingly with the allowed motion path, in several sub-classes also depending to their age (burn-up) averaged on a given burn-up interval. For sake of simplification, without loosing in significance of results, in this preliminary study, a simplified fuel composition has been assumed for each pebble, which takes into account an average fuel depletion and fission product build-up.

Depletion computations have been performed using the MONTEBURNS probabilistic chain [**3**] that uses, as calculation engine, the Monte Carlo code MCNP [**4**], which computes the neutron fission and capture rates in a number of radial and axial sub regions. The results were furnished as input for the Monte Carlo Code DISLOC [**5**] developed for determining the pebbles configurations induced by the random motions.

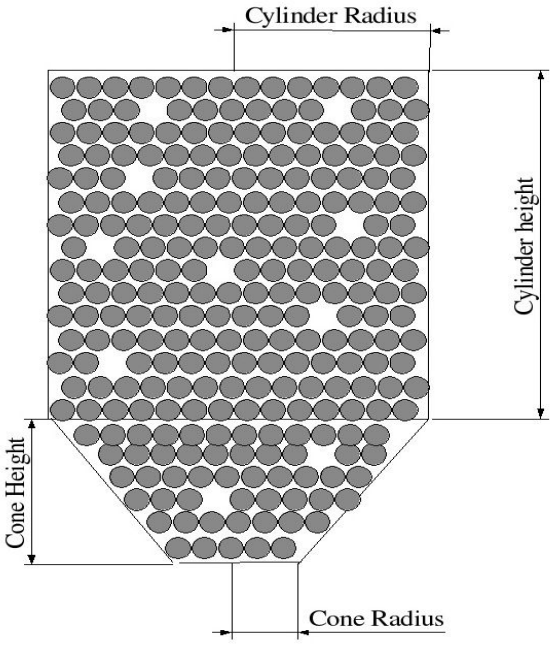

Figure 1. Schematic view of the PB-MR geometry definitions inside the DISLOC Code

2. The DISLOC Code

The pebbles were arranged, as in crystals, in a compact cubic lattice (using the crystallographic nomenclature) that, depending on the energetic constraints, shows a given amount of structural defects (i.e. vacancies, interstitial substitution, stacking fault, dislocations) and volume occupancy. The diffusion of the pebbles through defects is basically generated by weight and frictions forces. The elementary motion is the position exchange between a pebble and an adjacent vacancy (hop). In order to define the proper Transition Function, the hop probability of a pebble to a vacancy must be defined as:

$$f_p(\,[i,j,k] \text{--> } [i',j',k']) = f_v([i,j,k] \text{<-- } [i',j',k']).$$

Where the position [i,j,k] (and [i',j',k']) referenced to N(M), the set of pebbles positions (to V(M) the set of vacancy positions, respectively) at the time step M. The transition probability (TP) f_p for a pebble, from a given position [i,j,k], hops to the vacancy adjacent position [i',j',k'], is equivalent to the f_v form which expresses the probability of the same

event from the vacancy point of view. We assume that vacancies are randomly distributed, cannot exchange their position nor annihilate each other.

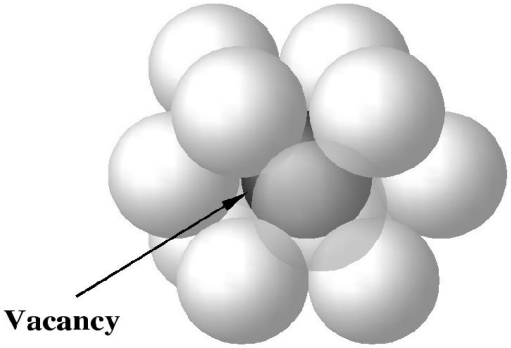

Figure 2. The vacancy first neighbors inside the PB-MR bulk.

In force of this assumption the f_v (or f_p) could be non-zero only for the adjacent pebbles of a vacancy (see fig. 2) and zero otherwise. A practical expression for the TP is in form of a Transition Matrix (TM) between a vacancy and the pebbles surrounding it. As illustrated in figure 2, the maximum number of "first neighbors" position is 12. This arrangement is highly probable for vacancies located in the system bulk, whereas vacancies located in contact with the geometrical border of the core show fewer neighbors than in the bulk. The elements of the TM are positive non-zero only for the position inside the geometrical border. Table I reports the TPs for an isolated bulk vacancy.

Table I. Tp values for the neighbor pebbles of a bulk vacancy(+)

Pebbles Neighbors	***TM bulk value***
Upper plane (k'+1)	0.92567
Same plane (k')	0.07360
Lower plane (k'-1)	0.00073

(+)TM values for the neighbor pebbles of a bulk vacancy. The network arrangement allows evaluating the vacancy – pebbles swap for 12 positions: 4 in the plane above vacancy, 4 in the same plane and 4 in the plane below. The values reported here are referred as the probability of the vacancy- pebble swap on each plane. The downward motion of vacancy is considerably less probable than the upward ones.

DISLOC simulates the pebble movements per time step (Discrete Time kinetic Monte Carlo) [**6**]. A DISLOC time step is defined as the complete cycle of evaluation of the TMs associate with the actual number of vacancies. From this definition the time steps are, in general, not homogeneous. The formation of pebble clusters with lower than average burn up level is of interest to hot point studies. For the demonstration purposes of this presentation, we simplified the burn up calculations, considering the flux burn-up evolution

during a given time interval in a number of sub-regions, as specified in Fig.3. From that, the elementary burn-up increase per sub-region of each travelling pebbles is determined and associated with the given time interval. These elementary burn-ups are added to the accumulated value of the pebbles according to the sub regions in which they transit.

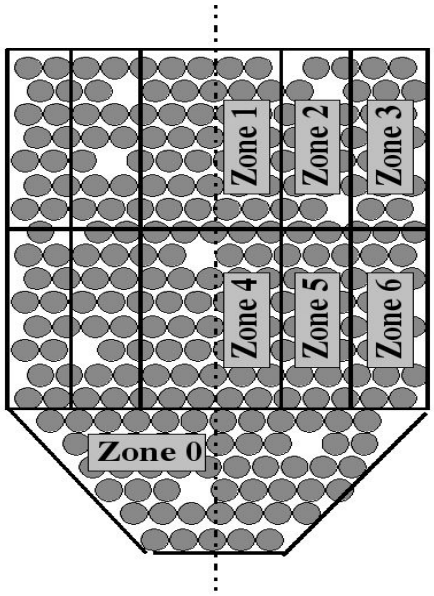

Figure 3. The six burn up zones on the PB-MR DISLOC Models. The burn-up rate of each zone is determined by a coupled MONTEBURN-MCNP calculation.

A "First In First Out" (FIFO) banking algorithm ensures pebbles supply in the system. The pebbles discharged from the bottom of the system and above the user defined burnup threshold, were banked in the FIFO buffer. When a vacancy reaches the top of the cylinder a pebble must replace it. The entering pebble would be take from the FIFO buffer while not empty, otherwise a new fresh pebble is introduced.

3. Calculations

In order to test the code capabilities two different PB-MR systems were considered. The first one is a small PB-MR containing a limited number of pebbles (628). In this case the calculation time is shorter, allowing a complete analysis of their burn up histories. The second one is a large, more realistic, PB-MR (28.083 pebbles), requiring a much larger computation time. It takes about 50 hours on an ALPHA processor to execute 500 time steps. Table II gives the geometric characteristics of the two simulated systems. It is worth noticing that, despite the large difference in the pebbles content, the two systems are big enough to show comparable behaviors with respect to the spatial short range of the TM under evaluation.

Table II. Comparisons of the Main input parameters for the two studied cases.

Input Parameter	*Small PB-MR*	*Large PB-MR*
Cylinder Height (cm)	50	180
Cylinder Radius (cm)	25	90.1
Cone Height (cm)	25	36.94
Bottom Cone Radius (cm)	6	25.04
Cone Aperture (degrees)	37.23	60.41
Number of Pebbles	628	28083
Number of Vacancies	9	839
Time Step	6000	500
Time step value (min)	4320	4320
Bur Up limits (%)	10.00%	10.00%

Since in this exercise we have limited our interest to the relative differences between accumulated burn-ups of pebbles at central and peripheral positions, their burn-up has been fictitiously accelerated by associating a larger amount of time to each time step. The main advantage of this assumption was the reduction of the computation time, in the hypothesis that the burn-up differences are independent from the discharge rate.

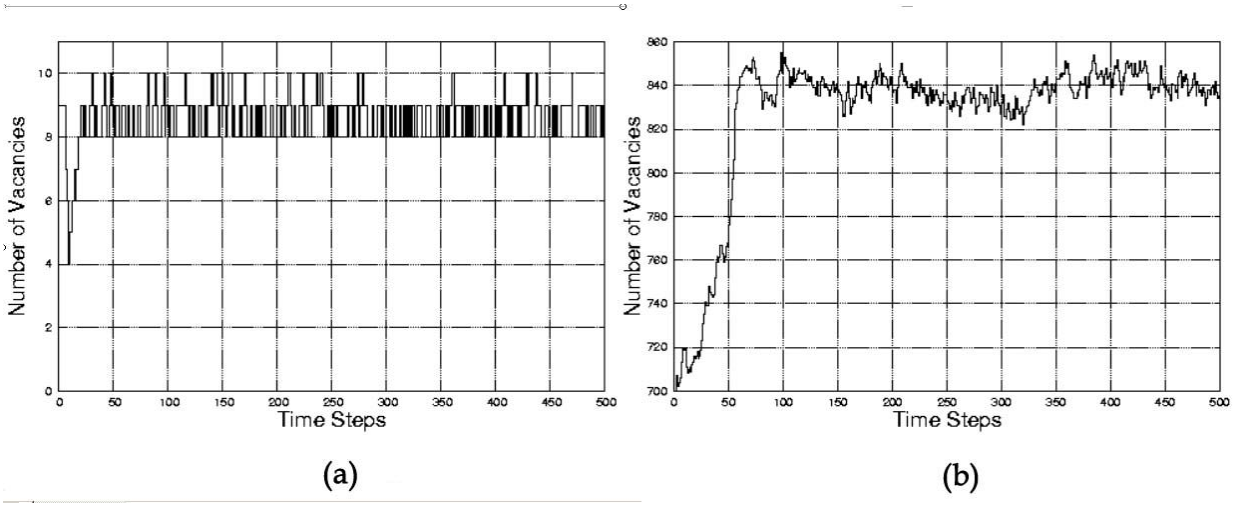

Figure 4. Averaged number of vacancies versus time step: a) Small PB-MR model. b) Large PB-MR model. In each case a certain amount of time steps is required to stabilize the averaged number of vacancies.

4. Results

As shown in figure 5, for both the simulated systems the average number of vacancies reaches an almost stationary value after a given number of time steps. The larger the system the larger is the number of time step required to stabilize the average number of vacancies. Figure 6a illustrates the burn-up evolution during the simulation of the small PB-MR system. After a first time interval, during which the burn-up increases homogeneously in all zones, it begins to differentiate in the lower zones 4-6 (see figure 3).

Table 3 Results

Zone	*Burn up per time step*	*Number of positions available in zone*	*Average number of pebbles in zone*	*Permanency (Average number of time steps in zone)*
0	0	59	56.38	26.231
1	1.61E-008	41	40.2	52.009
2	1.47E-008	146	144.02	72.632
3	1.17E-008	124	123.02	123.50
4	1.99E-008	34	32.93	34.090
5	1.78E-008	98	96.7	76.230
6	1.40E-008	135	134.11	147.37

The lower zones, where the burn up is low, reach a plateau of roughly 8%, whereas the upper zones burn up continues to grow until the limit value of 13% is reached. The introduction of fresh pebbles lowers the burn-up with different modalities in the various zones. The maximum burn-up is in zone 2.

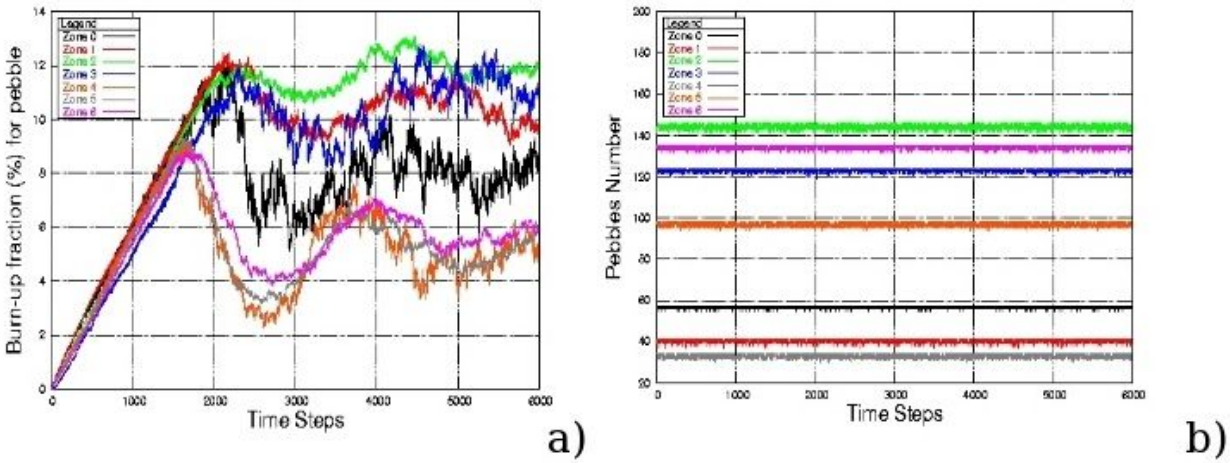

Figure 5. Small PB-MR models: a) Burn up vs. time step in the different zones. b) Number of Pebbles vs. time step in each zone.

Finally figures 6b (and Table III) shows that the number of pebbles (and vacancies) hosted in each zone is practically constant during the entire simulation. This fact clearly indicates that a stationary state, in which all the configurations are equivalent from the ergodic point of view, is reached and the hypothesis that burn up differences were independent from the discharge rate is qualitatively verified.

Conclusion

The preliminary phase of the DISLOC test has shown that the code is mature to leave the prototyping phase. The actual version of the program in entirely written in the OCTAVE [7] interpreted language that allows a good tuning of the algorithm and a carefully choice of the level of recursion for function and macros. In the case of real scale geometry the code is not fast enough for exploring a sufficiently large number of time steps. Work is in progress for optimizing the inner calculation cycle and I/O activity so to improve the execution speed. Furthermore, the possibility of implementation on a parallel machine is under study. For what concerns the proper choice of the parameters to be used in DISLOC, this could be realized if some specific information would be available on the relative pebble movements in some experiment (with fresh pebbles, at cold conditions). This information is necessary for properly tuning the DISLOC parameters.

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