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Monte Carlo burnup code development based on multi-group cross section method

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ABSTRACT

A multi-group cross section method was developed based on MOBAT code to save computing time. First, three PWR pin cell benchmark cases were computed by MOBAT, MCODE and SCALE. The results of the separate benchmark cases are consistent with each other; the maximum deviation of reactivity at a burnup depth of 100 MWd/kgU is less than 600 pcm, and the difference in nuclide concentrations is within 5%. Next, the same benchmark case was calculated by MOBAT using the multi-group cross section method. The results indicate that the method can give credible results while greatly reducing the computing time. Comparing the original MOBAT benchmark case to the results of the multi-group cross section method, the reactivity difference at a burnup depth of 100 MWd/kgU is about 100, the difference of nuclide concentrations is within 1%, and computation time was 3.5 times faster.

1. Introduction

Due to its effectiveness and accuracy, the use of burnup code coupled with Monte Carlo transport programs is widely developed around the world. Examples include INEEL's MOCUP (Moore et al., 1995) and MCWO (Chang, 2005), MIT's MCODE (Xu et al., 2002), Los Alamos's Monteburns (Trellue, 1998), and THU's RMC-DEPTH (She et al., 2013). The processing of cross sections is an important task for burnup codes. In the early days, researchers mainly paid attention to the time-averaged treatment of cross sections, as seen in the half step method (Yu et al., 2003) and prediction-correction method (Xu et al., 2002).

Today, more attention is paid to improving the computation time of burnup codes. Online processing of cross sections with continuous-energy Monte Carlo code is time-consuming. The amount of time is assumed by a binary search of cross sections, and is generally directly proportional to the number of burnup regions and nuclides present, as their energy meshes are inconsistent (Haeck and Verboomen, 2007). Unionized energy grid construction (Haeck and Verboomen, 2007; Leppänen, 2009) of cross sections favors the reduction of repetitive searches for the sake of reducing computation time. However, to obtain a refined and accurate unionized energy grid, the number of grid points required greatly increases, meaning more computational memory is necessary. This problem also occurs when using the doubling indexing (DI) method (Leppänen, 2009) for accelerating the energy grid search. The Computational Expense Oriented (CEO) and Energy Bin (EB) methods proposed by Liu et al. (2011) are good ways to improve computational speed and keep memory usage low. Even so, cross section searches and tallies frequently account for a significant portion of CPU time.

Separating cross section processing from the neutron transport calculation is a new attempt to accelerate the burnup computation. Fiorito et al. (2013) puts forward linear polynomial interpolation to predict time-dependent cross section curves and has demonstrated some acceptable results in a REBUS benchmark. Since the prediction is based on the hypothesis of linear change, it may be not suitable for nuclides with significant space self-shielding effects and cases with a large neutron spectrum difference.

To make the cross section predictions more reasonable and universal, we will introduce a Multi-Group cross section Method (MGM) in this paper. The multi-group cross section will be processed at the beginning of burnup, with the one-group cross section at each time step obtained from the weighted average of the neutron spectrum of the same energy grid. The method is valid when the multi-group cross section is unchanged with burnup. This assumption could be guaranteed if the energy-group number and grid are close to point-wise nuclear data, as seen in Haeck and Verboomen (2007). However, it may be not necessary to build such elaborate energy group structures, as the initial processing of multi-group cross sections takes into account the

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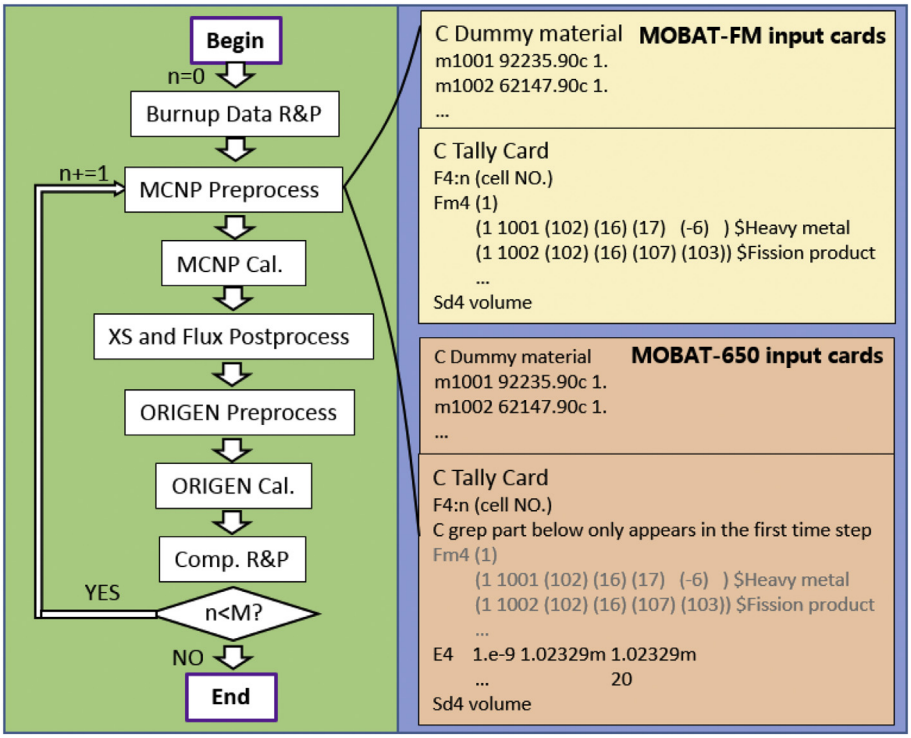

Fig. 1. MOBAT flow chart and input card examples for flux multiplier method and 650 groups method.

resonance cross section processing of an objective model. An important focus of this paper is to determine what energy group structure and energy spectrum change can achieve acceptable one-group cross sections. These steps are expected to greatly reduce computation times, as an energy spectrum tally for each burnup region has low computational requirements.

In this paper, we first introduce the accuracy of conventional burnup code MOBAT (Zhu, 2015) developed by Shanghai Institute of Applied Physics (SINAP). From the benchmark case, comparisons will be made to calculations employing MOBAT with the multi-group cross section method, specifically comparing the neutron multiplication factor, main cross sections, and major nuclides evolution. Section 2 includes our methodology and a code flowchart introduction. Section 3 is results and analysis, and section 4 contains our conclusions.

2. Methods and code flowchart

The MCNP (Briesmeister, 2010) and ORIGEN (Croff, 1980) coupled burnup code with Batch language (MOBAT) is a fuel management code developed by SINAP. MOBAT consists of several modules, a flow chart shown in Fig. 1, demonstrates these modules and shows how MOBAT functions.

The burnup information, including power, time step, time number, material, and volume, is embedded in the MCNP input file using a specific command and format. The code first reads that information and removes commands.

Next, it generates dummy material and tally multiplier cards in the input file. By default, 90 fission products and 39 actinides are tallied in each burnup region. The nuclide compositions are not changed in the first time step, and are updated from the ORIGEN output file in the following time steps. It should be emphasized that the densities of burnup material in the MCNP input file must be modified since not all nuclide ratios are preserved. Finally, the code calls the MCNP executive program and outputs the neutron multiplication factor and reaction rates.

In the post processing module, the flux and one-group cross section can be obtained. The flux multiplication factor (FMF) is calculated by the following equation:

$$FMF = \frac{p}{\sum_{i=1}^{n}\sum_{j=1}^{m_i} N_{ij}\left[\int \sigma_{ij,f}(E)\phi_i(E)dE\right]V_i Q_j} \quad (1)$$

P is the input power [MW]; N_{ij} is the atom density [1/barn-cm^3] of the j-th nuclide in the i-th burnup region, $\sigma_{ij,f}(E)$ is the microscopic fission cross section of N_{ij}, $\varphi_i(E)$ is normalized flux in the i-th burnup region tallied by MCNP code, V_i is the material volume in the i-th burnup region, and Q_j is the recoverable energy of the j-th nuclide, calculated by following equation:

$$Q = 1.29927 \times 10^{-3}(Z^2A^{0.5}) + 33.12 \quad (2)$$

Here, Z is the atomic number of the nuclide and A is the mass number.

The actual flux is $\varphi_i(E)$ multiplied by the FMF. The one-group cross section is the tallied reaction rate divided by $\varphi_i(E)$.

In the ORIGEN preprocess module, several input files need to be created and updated. The nuclear data file TAEP9.INP is updated with the calculated one-group cross sections. The flux and time step are updated in the command file TAPE5.INP. Irradiation for specified Flux (IRF) must be used as the burnup command instead of Irradiation for specified Power (IRP) in TAPE5.INP, as the local power in the multi-region burnup calculation usually changes with time greater than flux, and IRP is not suitable for non-fuel material. The concentration input file TAPE4.INP is inherited from the last time step concentration output file, TAPE7.OUT.

After that, the code calls the ORIGEN executive program and outputs the evolved nuclides. Additionally, the code calculates the value of burnup depth.

Finally, if the iteration number n is lower than the pre-set time step number M, the code moves on to the next time step computation. Otherwise, it exits the program and finishes the burnup calculation.

If using the multi-group cross section method, some modules should be amended.

In the MCNP preprocess module, for the first time-step, the reaction rates are tallied with a specified energy grid and processed into multi-group cross sections. For other time-steps, only specified energy-group