Development Status of MCS as Cross-section Generation Tool for Fast Reactor Analysis

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1. Introduction

The methods used in the MCS Monte Carlo (MC) code to generate multi-group (MG) cross-section (XS) for nodal diffusion simulator calculations are described in this paper. Previous research [1, 2] focused on few-group XSs, scattering matrices, diffusion coefficients homogenized in infinite, and leakage-corrected critical spectra. The primary goal of this paper is to provide brief insight into the development status of MCS, which incorporates an additional feature of the automated burnup sequence that was recently implemented for the managing of restart calculations with branch variations. This feature enables XSs to be parameterized (known as case matrix) to cover the entire range of local operating conditions, including fuel temperature, water/coolant temperature and density, and/or boron concentrations, in a single run, which is required for thermal hydraulic feedback and burnup calculations.

2. Methods used for spatial homogenization and branch calculations

The primary objective of spatial homogenization is to preserve the local reaction balance when XSs collected from the local heterogeneous transport calculations (assembly-level) are utilized as basic components for the global homogeneous system (core-level). In formal terms, the homogenization of XS Σ_g is as follows:

$$\Sigma_g = \frac{\int_V d^3r \int_{E_g}^{E_{g-1}} dE \Sigma(r,E)\phi(r,E)}{\int_V d^3r \int_{E_g}^{E_{g-1}} dE \phi(r,E)}, \quad (1)$$

where ϕ is the scalar flux, and the integration is performed over the volume of the homogenized region and energy group g. The spatial dependence of Σ reflects the geometry's heterogeneity, even though it mainly consists of discrete uniform material zones. Spatial homogenization, in particular, entails averaging the physical continuous energy XSs over volume and flux spectrum. [1, 2] provide more information on spatial homogenization.

For depletion calculations, the microscopic XS of nuclides in the fuel material is required, and the micro XS of nuclide x is defined as:

$$\sigma_{g,x} = \frac{\int_V d^3r \int_{E_g}^{E_{g-1}} dE \sigma_x(r,E)\phi(r,E)}{\int_V d^3r \int_{E_g}^{E_{g-1}} dE \phi(r,E)}, \quad (2)$$

where x is the nuclide index and the user can determine the number of nuclides required for burnup calculations, which depends on the selected burnup chain that is used in the certain nodal diffusion simulators.

Furthermore, MCS provides an automated burnup feature for branch variations that considers changes in operating conditions, including fuel temperature, moderator/coolant density and temperature, and/or boron concentration. Variations in the thermal hydraulic state can be accounted for by changes in material temperatures and densities. When the automated calculation feature is executed, the code generates another output file in which the XS data is structured in a manner that processing scripts can easily accessed. The user can determine which parameters are included in the output.

3. Verification on lead-bismuth-cooled fast reactor ANTS-100e

Fig. 1 [3] depicts the ANTS-100e core design layouts. The active core consists of 138 fuel assemblies (FAs) that are divided into two enrichment zones of 10.0 and 13.0% uranium nitride. Each FA has four axial components: a lower reflector, fuel, a gas plenum, and an upper reflector. Each 75-cm axial reflector is made of stainless steel, and the gas plenum is 75 cm long, which may compensate for ANTS-100e's fission gas release. There are two separate control rod systems: a primary system and a secondary system, each with three and nine control assemblies. The equivalent active core size is 235 cm in diameter and 100 cm in height, resulting in a height/diameter ratio of 0.43.

The typical computation procedure for nodal FR whole-core analysis is depicted in Fig. 2. In this work, the MC code MCS is used to generate the MG XS, which is then fed into the nodal diffusion code RAST-F (RF) [4] for 3D core simulation. The 24-group energy structure has been used, which is a subset of the 33-group structure of the ECCO-33. Because of significant statistical uncertainties in neutron flux for the last ten groups of the ECCO-33 when using the MC method, the 24-group structure is created by combining the last ten thermal energy groups into a group. A standard framework for obtaining the 24-group XSs for every fast reactor component is addressed in [2, 4]. If thermal hydraulic feedback is required, the branch calculations in this fast

reactor can be performed with two variations of fuel temperature and coolant density.

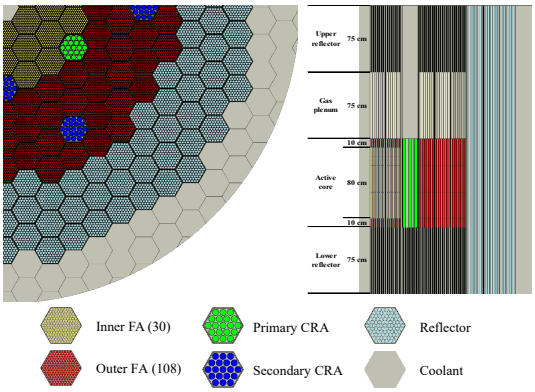

Fig. 1. Radial and axial layouts of the ANTS-100e quarter core.

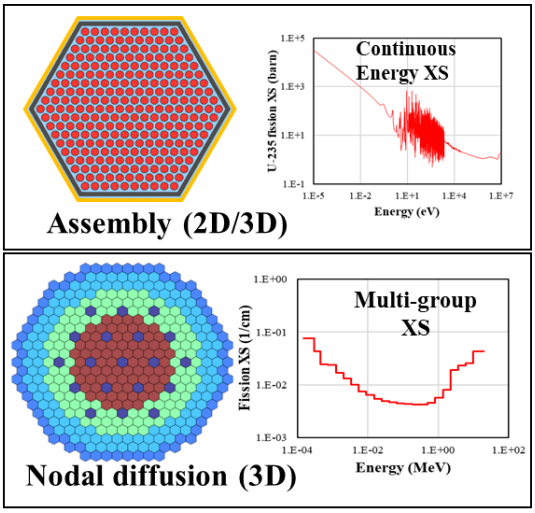

Fig. 2. Typical computation procedure for coarse-mesh FR whole-core calculation.

The depletion calculation without thermal hydraulic feedback is performed in this work using the two-step code MCS/RF and the standalone MC MCS code as reference. The burnup chain for 221 actinide and fission products is opted, resulting in the preparation of microscopic XS of 221 nuclides by MCS. The fuel temperature and lead-bismuth coolant density are set at 750K and 10.24 g/cm^3, respectively. The temperature interpolation feature is available in MCS for temperature points that do not exist in the data library.

A single 2D FA model with reflective BCs is used to calculate the FA XSs by MCS. The homogenized XS for non-multiplying zones, such as control rod and axial components located far away from active core, is scored with the 2D supercell models. To properly account for neutron leakage, the XS for the radial reflector assembly and its nearby FA is generated using the radial reflector model, in which the vacuum boundary condition is applied on the right side of the model. The motives for such separation are clearly stated in [2]. The execution time is expected to be longer than the normal one with only macroscopic XS due to the large number of nuclides and the huge number of histories required for accurate microscopic XS. Non-fuel materials do not require microscopic XS data. Furthermore, because it is assumed that the XS in fast reactors seems to be insignificantly burnup-dependent, the XS for all components is only produced at the beginning-of-cycle (BOC). Further research should be done to investigate how the neutron spectrum changes with burn-up.

ENDF/B-VII.0 library is utilized in all MCS simulations. As a reference, the MCS pin-wise depletion calculation is performed with 5 inactive batches, 20 active batches, and 1,000,000 particles per batch at full power and with all rods out. There is a total of 233,220 burnup cells in MCS. The total burnup time is ten years, and the burnup time step is 0.5 year, for a total of 21 burnup points, resulting to the average burnup of 45.32 MWd/kg. The CRAM solver is incorporated in MCS to solve the Bateman equation and is optimized to take advantage of the sparsity of the burnup matrix to reduce computation time [5]. The burnup chain could include up to 4,060 isotopes from the ENDF decay library, but MCS only uses more than 1,600 of those isotopes by default. The semi-predictor/corrector (semi-PC) method is adopted in MCS burnup calculation for improving the stability of the established MC burnup calculation.

RF simulates a full-core assembly-wise simulation; each FA is divided into 20 axial meshes (active height only), resulting in a mesh size of 5 cm. As a result, RF has 2,760 depletion zones. The burnup calculation for the fast reactor in RF is based on the CRAM module solving the transmutation equation [4]. Notably, the current version of RF does not support either PC or semi-PC method.

Fig. 3 shows the core k_{eff} as a function of burnup obtained by MCS/RF and MCS, and the eigenvalue difference during depletion is shown to be within 50 pcm during the few burnup steps at the BOC since the amount of fission products does not significantly build up. At the end-of-cycle (EOC), the difference becomes more noticeable. Such difference could be attributed to i) the use of MGXS, ii) a burnup chain of 221 nuclides, which is significantly lower than the MCS burnup chain, and iii) the incapability to use the PC method, which possibly overestimate the fission product buildup during depletion. Indeed, additional MCS burnup curve shows better agreement with the MCS/RF solution when not using the PC method.

MCS/RF and MCS depletion calculations can provide isotope-wise number densities for a desired depletion chain with respect to the burnup steps. The mass inventories of several major fuel isotopes over the burnup are shown in Fig. 4. The isotopes of interest are ^{235}U, ^{236}U, ^{238}U, and ^{239}Pu. Notably, there is a high degree of agreement between MCS/RF and MCS in the inventory of major heavy nuclides, either semi-PC or no

PC is used in MCS. Further investigation is required to clarify the difference in k_{eff}.

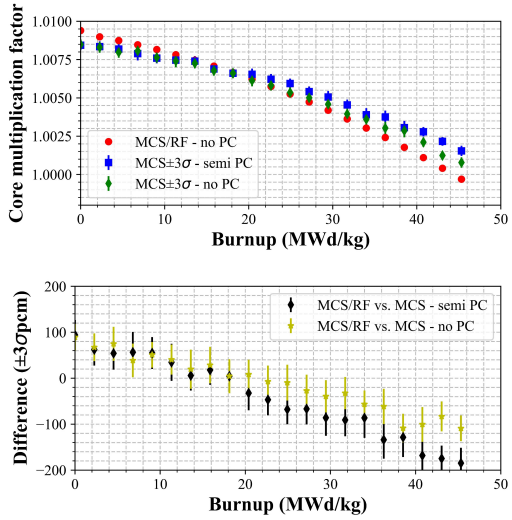

Fig. 3. Core multiplication factor as function of burnup, MCS/RF vs. MCS (to be updated).

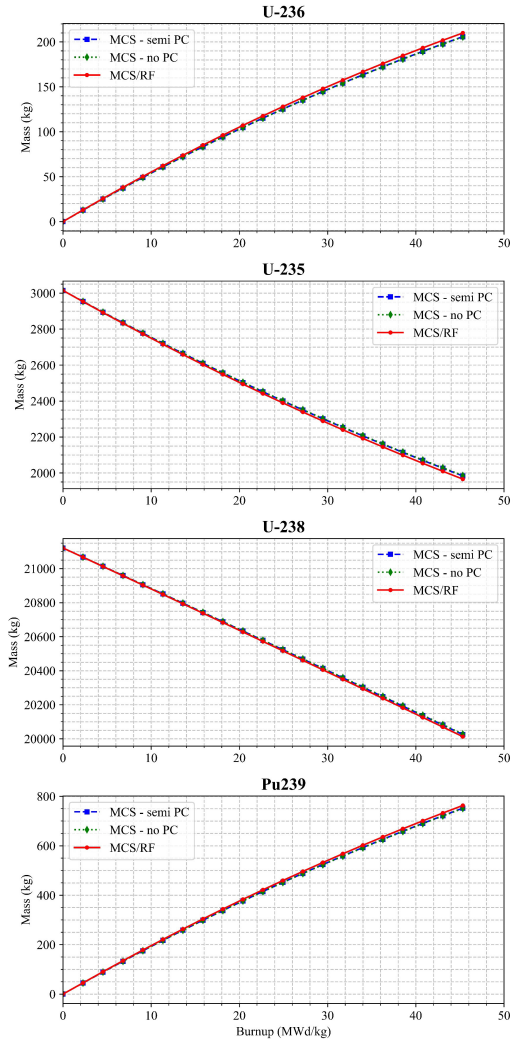

Fig. 4. Major nuclides mass inventory.

Fig. 5 shows the in normalized radial power profiles at BOC, middle-of-cycle (MOC, at 22.66 MWd/kg) and EOC (at 45.32 MWd/kg) by MCS/RF, whereas Fig. 6 illustrates the local relative difference in radial power between MCS/RF and MCS. The comparison in axial power is shown in Fig. 7. To reduce power uncertainty, the criticality calculation for each burnup point must be restarted with relatively high neutron histories; and the MCS maximum standard deviation in radial and axial power is less than 0.4% and 0.1%, respectively. Table I summarizes the maximum and root-mean-square (RMS) radial assembly power and axial power difference between MCS/RF and MCS at three burnup points. Notably, the MCS/RF power profiles appear to agree with MCS standalone solutions.

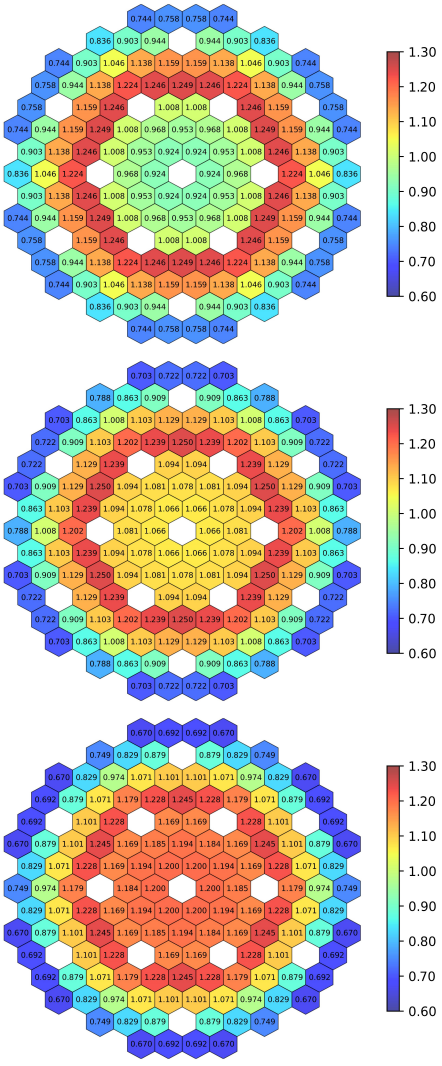

Fig. 5. Radial power distribution at BOC, MOC and EOC (top to bottom) by MCS/RF.

Table I: Summary of radial power differences, MCS/RF vs. MCS.

Power diff. (%)	BOC	MOC	EOC
|Max.|	0.92	1.06	1.09
RMS	0.40	0.44	0.42

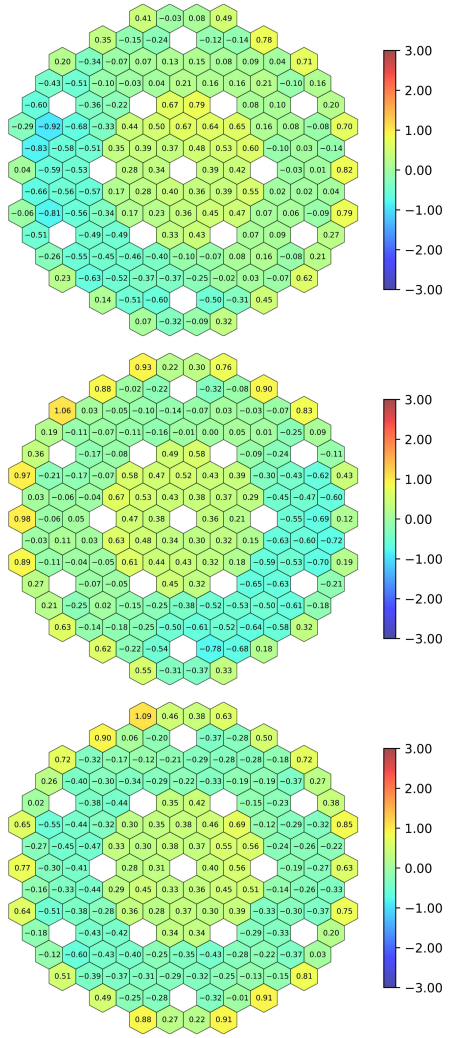

Fig. 6. Difference in radial power distribution at BOC, MOC and EOC (top to bottom), MCS/RF vs. MCS.

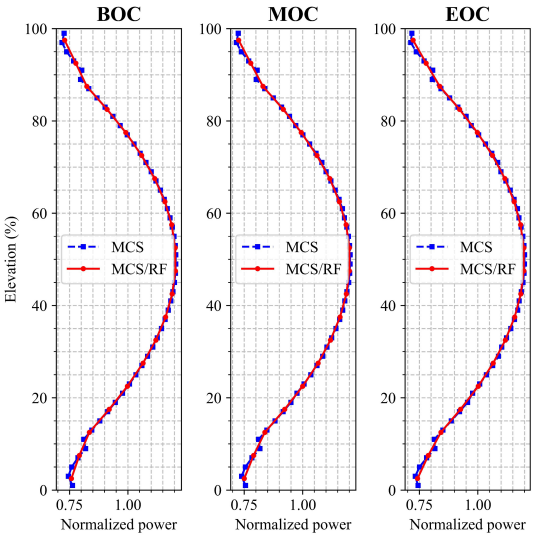

Fig. 7. Axial power distribution at BOC (left) and EOC (right), MCS/RF vs. MCS.

4. Conclusions

The MCS MC code has been utilized to generate MG XS for nodal diffusion simulator-based fast reactor simulations, and the procedure has been validated in terms of core depletion calculation accuracy. In a FR whole-core study, RF performs depletion simulations on 24-group XS to estimate core multiplication factor and power profiles in order to evaluate the MG XS generation capability in MCS. During the burnup cycle, the k_{eff} difference between MCS/RF and MCS is less than 200 pcm, and the maximum and RMS differences in radial power are less than 1.1% and 0.45%, respectively. To improve solution accuracy, the burnup chain in RF should be optimized, and the PC or semi-PC algorithm should be implemented. Further research should focus on estimating the reactivity feedback coefficients and control rod worths by MCS/RF at various burnup points. More branch calculations should be performed and validated in associated with thermal hydraulic feedback calculation. Finally, the findings of this study indicate that the MCS could be a reliable tool for generating MG XS for fast reactor core analysis.

Acknowledgement

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