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Verification and Validation of 0-D Transmutation Capabilities in OpenMC Using Fusion-Relevant Benchmarks

Neutron irradiation of materials within a fusion device results in the production of a wide variety of transmuted nuclides. Knowing the resulting material composition is essential for predicting nuclear properties such as decay heat, activity, gamma emission, dose rate, and waste categorization. Nuclide inventory tracking simulations are complex due to the large number of nuclides, intricate decay chains, and vast differences in half-life time scales. This simulation becomes particularly challenging in the fusion context due to the higher energy of fusion neutrons, which increases possible reactions. OpenMC's depletion capability has previously been used alongside neutron transport simulations to obtain reaction rates. Previous studies have shown good agreement between OpenMC's coupled transport depletion and Serpent's, which also supports integrated transport and depletion capabilities. Additional comparisons have demonstrated good alignment with experimental data using fusion-relevant neutron spectra highlighting OpenMC's reliability in a fusion context. The authors have recently implemented support in OpenMC for stand-alone 0-D transmutation, allowing the use of a multigroup flux instead of transport-derived rates. This enables direct comparison with 0-D transmutation codes such as FISPACT-II, ORIGEN, ALARA, and ACAB. In this study,we compare OpenMC 0.15.3 results to those produced by the 0-D transmutation code FISPACTII. We present comparisons of decay heat predictions against data from 132 irradiation experiments performed at the Fusion Neutron Source. These experiments include a broad range of elemental targets and fusion-relevant materials irradiated with 14 MeV neutrons and are part of the openaccess CoNDERC benchmark suite. The results show good agreement between the experimental measurements, FISPACT-II, and OpenMC in the majority of cases. Elements exhibiting the largest discrepancies (In, Ir, Rh) highlight areas where further refinement of OpenMC's depletion capabilities is needed. This work identifies specific nuclides and transmutation pathways where discrepancies remain relative to FISPACT-II, helping to guide future development. While OpenMC's 0-D transmutation capabilities have improved, further work is needed in the areas of simulation accuracy. This study provides a valuable benchmark for tracking the progress of OpenMC's depletion features in the context of fusion applications for current and future OpenMC releases.

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