Isomeric Branching and GENDF XS in OpenMC Deplete

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Full treatment of isomeric branching is important in predicting activation in high yield fusion generators. Here-to, OpenMC[1] Deplete lacked energy dependent isomeric branching. Rather, pre-processed fixed branching ratios (BR) were stored for reactions on the chain. This work will present implementation of full energy-dependent isomeric branching in OpenMC, accomplished by leveraging UKAEA GENDF[2] activation libraries. These libraries are ENDF evaluations processed into group-averaged form by PREPRO, with partial cross-sections (XS) to each isomeric product consolidated on MF=10. The implementation is ultimately applied to Helion's currently operational fusion prototype, Polaris.

First an augmented OpenMC chain is produced, reactions with isomeric branching flagged and GENDF excited states matched with decay metastable states. During deplete, multi-group flux with GENDF energy structure is tallied. When a pathway with a BR flag is encountered a helper fetches the GENDF MF=10 XS. The flux and partial XS are collapsed, forming BRs. These are applied to the reaction rate, unfolding it into multi-target isomeric pathways.

With this GENDF groundwork, further enhancements were made beyond BR.

1. GENDF XS as the activation XS, in-lieu of the continuous energy transport XS. Benefits:
    a. wider nuclide coverage (especially metastables)
    b. faster transport solve and XS collapse (albeit coarser energy structure)
2. Addition of MT=4 (n,n') neutron inelastic activation. Previously absent without the requisite pipework for isomeric pathways e.g. no In115(n,n')In115m products.

CoNDERC FNS Decay-Heat Benchmark[3] results will be presented. Improvements are stark:

a. significantly improved agreement with experiment
b. near perfect agreement with FISPACT-II[2]

[1] P.K. Romano, N.E. Horelik, B.R. Herman, A.G. Nelson, B. Forget, K. Smith, "OpenMC: A state-of-the-art Monte Carlo code for research and development", Annals of Nuclear Energy, vol. 82, pp. 90–97, 2015. DOI: 10.1016/j.anucene.2014.07.048

[2] J.-Ch. Sublet, J.W. Eastwood, J.G. Morgan, M.R. Gilbert, M. Fleming, W. Arter, "FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling", Nuclear Data Sheets, vol. 139, pp. 77–137, 2017. DOI: 10.1016/j.nds.2017.01.002

[3] M.R. Gilbert and J.-Ch. Sublet, "Experimental decay-heat simulation-benchmark for 14 MeV neutrons and complex inventory analysis with FISPACT-II", Nuclear Fusion, vol. 59, 086045, 2019. DOI: 10.1088/1741-4326/ab278a. Dataset: https://nds.iaea.org/conderc/fusion/

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