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Development of a set of benchmark problems to verify numerical methods for solving burnup equations

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ABSTRACT

A comprehensive set of transmutation chain benchmark problems for numerically validating methods for solving burnup equations was created. These benchmark problems were designed to challenge both traditional and modern numerical methods used to solve the complex set of ordinary differential equations used for tracking the change in nuclide concentrations over time due to nuclear phenomena. Given the development of most burnup solvers is done for the purpose of coupling with an established transport solution method, these problems provide a useful resource in testing and validating the burnup equation solver before coupling for use in a lattice or core depletion code. All the relevant parameters for each benchmark problem are described. Results are also provided in the form of reference solutions generated by the *Mathematica* tool, as well as additional numerical results from MATLAB.

1. Introduction

Nuclear fuel undergoes constant and significant change during operation with criticality, radioactivity, and material performance all affected as a result. The formation of new isotopes following the absorption of a neutron in the fuel causes power shifts and flux profile changes; consequently, these phenomena need to be monitored to ensure safe and efficient reactor operation. Computationally, these events are simulated using lattice depletion codes – a catch-all term for the coupling of a neutron transport solver and a burnup equation solver.

Traditionally, burnup solvers are developed with the purpose of ultimately being coupled with an established neutronics solver. With very little in terms of standalone burnup solvers openly available, the lack of benchmarks to verify these solvers has become apparent. Before these burnup solvers can be used confidently to acquire the numerous parameters important to core life-cycle analysis, they must be thoroughly vetted to ensure sufficiently accurate solution methods.

This study presents a set of benchmark problems developed for the verification of existing and new standalone burnup equation solvers. These benchmarks were specifically developed to challenge numerical solvers and help identify issues usually associated with burnup solver methods; e.g., matrix exponential methods and linear chain methods. The benchmarks are described in robust detail and results are presented for each problem as a resource for users to verify their own solvers and methods. The results include analytical solutions from the *Mathematica* package, as well as numerical results from MATLAB [3,5].

2. Development of benchmark problems for numerical verification of burnup solvers

The benchmark problems in this study were developed to verify the numerical methods in a burnup solver. Starting with a simple two-isotope system and building up to a complex decay/transmutation chain, these benchmarks incorporate numerous physical phenomena associated with burnup problems and are designed to verify the accuracy of a solver trying to address these important events. Numerous decay chains were chosen, with and without reactions and fission yields, over a wide range of decay probabilities. The problems were chosen with the purpose of challenging the methods in burnup solvers to ensure accuracy of solutions for any given set of isotopes. Specifically, the isotopes and the time steps chosen generated highly ill-conditioned problems, meaning the condition number of the matrix corresponding to the problem is very large. As such, these matrices are close to singular, consequently making the computation of a solution prone to large numerical errors [4].

Additionally, these problems were generated for the explicit purpose of testing burnup solvers, not the neutronics solvers they are generally coupled with in lattice depletion codes; namely, the method for solving the matrix problem is tested, not the method of generating the matrix given a transport solution. The following

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subsection briefly describes the isotopes tracked in each of the transmutation chains. Section 3 details the specific parameters needed to regenerate the solution to each problem.

2.1. Description of Benchmark problems

Benchmark problem #1 is a simple decay scheme – ^{238}U alpha decays into ^{234}Th, which then itself decays. While lacking complexity, this decay scheme tests any numerical method due to the wide range of half-lifes, leading to a highly ill-conditioned problem.

Table 1
Parameters for Benchmark #1.

Time step (s) = 5.00E+17		
	Initial concentration (atoms)	Half-life (s)
U-238	1.0000E+10	1.4099935680E+17
Th-234	0.0000E+00	2.082240E+06

Table 2
Parameters for Benchmark #2.

Time step (s) = 1.00E+12		
	Initial concentration (atoms)	Half-life (s)
Np-237	1.00E+12	6.7659494310E+13
Pa-233	0.00E+00	2.330640E+06
U-233	0.00E+00	5.023969920E+12

Table 3
Parameters for Benchmark #3.

Time step (s) = 1.00E+04		
	Initial concentration (atoms)	Half-life (s)
Pb-211	1.00E+10	2.1660E+03
Bi-211	1.00E+04	1.2840E+02
Tl-207	1.00E+01	2.8620E+02
Pb-207	0.00E+00	*Stable*

Table 4
Parameters for Benchmark #4.

Time step (s) = 8.64E+04			
	Initial concentration (atoms)	Half-life (s)	(n,γ) Rxn rate (s^{-1})
U-235	1.00E+12	2.2210238880E+16	1.0E−04
U-236	1.00E+02	7.390789920E+14	1.0E−04
U-237	1.00E+02	5.8320E+05	–
Np-237	1.00E+02	6.7659494310E+13	–

Benchmark problem #2 is another fairly simple decay scheme, but now introduces two types of decay – alpha decay and beta decay. This further tests the look-up schemes for the decay library in a burnup solver while still providing a wide range of eigenvalues to verify convergence to the correct solution.

Benchmark problem #3 is similar to the first two benchmarks, but the introduction of ^{207}Pb tests the ability of a matrix exponential method to identify and properly treat a stable isotope. In a matrix exponential method, a matrix of burnup coefficients called the transition matrix is generated. The transition matrix holds all the relevant parameters regarding the transmutation of each isotope – decay constant, reaction rate, etc. – and generally defines the condition of the problem. A stable isotope, such as ^{207}Pb, may introduce a zero element into the diagonal of the matrix, reducing the rank of the matrix to less than full and rendering the problem unsolvable. These elements need to be identified, reduced from the transition matrix, and solved for in a different manner.

Benchmark problem #4 follows the production of ^{237}Np via ^{235}U. This problem includes the decay of each isotope, but now incorporates reaction rates – specifically the (n,γ) reactions involved in producing ^{237}Np. This method tests the ability of a burnup solver to calculate and incorporate reaction rate branching ratios. Burnup solver algorithms need to be able to identify the relationship between each of the isotopes being tracked and properly implement the probability of one isotope decaying into another (branching ratios) via the information in decay libraries.

Benchmark problem #5 is a complex actinide chain following the decay and transmutation of ^{238}U. This problem includes a wide range of decay probabilities, reaction rates, and a closed decay loop from ^{244}Cm to ^{240}Pu.

Benchmark problem # 6 is an analytical benchmark problem that follows the production of a fission product important to reactivity – ^{135}Xe. This problem tests the methodology of calculating and incorporating fission product yields given an average incident neutron energy. Fissionable isotopes have fission yield probability data stored in the fission yield sublibrary of the ENDF/B libraries. For some isotopes, yields are available for multiple discrete energies of incident neutrons (thermal, epithermal and fast). Interpolating between these discrete energies is an important component of implementing fission yields.

2.2. Bateman equations

For each of the transmutation chains, an associated burnup equation is generated for each isotope in the chain. The collection of all the equations in each chain leads to a system of ordinary

Table 5
Parameters for Benchmark #5.

Time step (s) = 8.64E+05			
	Initial concentration (atoms)	Half-life (s)	(n,γ) Rxn rate (s^{-1})
U-238	1.00E+10	1.4099935680E+17	1.0E−04
U-239	1.00E+03	1.4070E+03	–
Np-239	0.00E+00	2.0355840E+05	–
Pu-239	0.00E+00	7.60853735110E+11	1.0E−04
Pu-240	0.00E+00	2.0704941360E+11	1.0E−04
Pu-241	0.00E+00	4.509581040E+08	1.0E−04
Pu-242	0.00E+00	1.178676360E+13	1.0E−04
Pu-243	0.00E+00	1.784160E+04	–
Am241	0.00E+00	1.3651817760E+10	–
Am-243	0.00E+00	2.325795120E+11	1.0E−04
Am-244	0.00E+00	3.6360E+04	–
Cm-244	0.00E+00	5.715081360E+08	–

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