#### Validation of Spent Nuclear Fuel Output by Cyclus, a Fuel Cycle Simulator Code

Gwendolyn J. Chee, Gyutae Park, and Kathryn D. Huff

Dept. of Nuclear, Plasma and Radiological Engineering, University of Illinois at Urbana-Champaign gchee2@illinois.edu

# INTRODUCTION

CYCLUS [1], a fuel cycle simulator, was used to simulate the United States' nuclear fuel cycle from 1967 through 2013. The spent nuclear fuel (SNF) inventory from the CYCLUS simulation was compared to the SNF inventory from the U.S Department of Energy (DOE) sponsored Unified Database (UDB) [2]. The UDB provides comprehensive and consistent technical data on reactor sites and SNF from the beginning of nuclear reactor operation in the United States until 2013. This comparison between CYCLUS and UDB establishes a realistic validation of CYCLUS' capability to produce total spent fuel mass and accurate isotopic compositions that closely match reality.

# BACKGROUND

CYCLUS is an agent-based fuel cycle simulation framework [3], which means that each facility in the fuel cycle is modeled as an agent. CYCAMORE [4] provides agents to represent process physics of various components of the nuclear fuel cycle (e.g. mine, fuel enrichment facility, reactor) [5]. The nuclear fuel assemblies tracked within the simulation are recipe-based. Recipes specify mass fractions for each isotope for fresh and spent fuel. They are calculated ahead of time using neutronics depletion analysis tools such as ORIGEN [6], then entered directly into the fuel cycle simulation [7].

## MOTIVATION

The United States is currently considering various nuclear fuel cycles and geologic disposal options [8]. Decisions such as waste package spacing, waste repository size and geometry will be influenced by key criteria such as thermal load of waste packages and the thermal capacity of the selected geologic host media. Waste package thermal evolution depends on the decay heat contribution from each isotope in the spent fuel. Therefore, to correctly simulate loading of a waste repository based on thermal constraints in Cyclus, the simulation must first give isotopic compositions and spent fuel masses that closely replicate reality.

# METHODOLOGY



Generating Cyclus Simulation and Analysis

A CYCLUS simulation of the United States nuclear fuel cycle was created using published data of the 112 commerical nuclear reactors that have operated since 1967 in the United States. The reactor deployment data was obtained from the Power Reactor Information System (PRIS) reactor database [9]. Relevant data includes country, reactor unit, reactor type, net capacity (MWe), first grid date and shutdown date. United States' reactor data was extracted and used to populate the Cyclus simulation. The recipes used in the Cyclus simulations are taken from a reference depletion calculation done using ORIGEN [6] for burnups of 51 and 33 GWDt/MTU. They were also used in [10, 11].

Jinja2 [12], a Python templating language, was then used in Python to render the data into an input file that is accepted by CYCLUS. The output file produced by CYCLUS was also analyzed using Python.

The assumptions made for this Cyclus simulation include:

- 1. Cycle time is assumed to be 18 months.
- 2. Refueling time is assumed to be 1 month.
- 3. There is isotopic decay.

#### **UDB** Data Analysis

The UDB database contains commercial SNF information from 1967 through 2013. Data such as initial enrichment, burnup, mass of spent fuel and discharged dates were collected from multiple sources [7]. Whereas a such as isotopic compositions, heat and activity were mined by performing irradiation and decay calculations on every fuel assembly based on the collected in the coll

The UDB dataset for this work included discharged fuel assembly data per reactor, specific isotopic concentrations and decay heat for each assembly along with its discharge date [2]. The UDB set was imported into Python, processed and compared Cyclus simulation output. All scripts and data used are available in [13].

## **RESULTS AND ANALYSIS**

The primary outcome of this validates to provide comparisons between CYCLUS data and UD venta for spent fuel mass and isotopic contributions to the spent fuel mass.

#### Cumulative Total Spent Fuel Mass Comparison

Figure 1 shows the cumulative spent fuel mass for both CYCLUS and UDB data from 1967 to 2013. The spent fuel mass estimated by CYCLUS is larger than UDB data before the year 2000 and diverges after, with UDB being larger. The discrepancies can be attributed to the provide the specifies refuel and cycle times for each reactor as constant in months. In reality, the cycle and refuel times vary the hout each reactor's lifetime and are not exact integer multiples of one month.

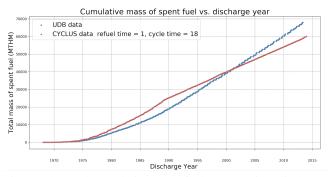


Fig. 1: The total cumulative spent fuel mass against discharge time for Cyclus and UDB data from 1967 through 2013.

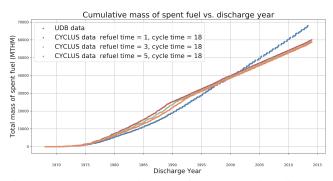


Fig. 2: The total cumulative spent fuel mass against discharge time for Cyclus and UDB data from 1967 through 2013 for various refueling times.

The Nuclear Energy Institute (NEI) reported that there has been significant variance in the refueling period for reactors in the United States. The average refuelling time in 1990 was 104 days, and generally decreased to an average refuelling time of 35 days in 2017 [14].

Figure 2 includes plots of total spent fuel mass from Cyclus simulations where refuel time is increased. A longer refuel time brings the temperature fuel mass from Cyclus simulations closer to the UDB data before 2000.

The larger cumulative UDB spent fuel mass compared to the Cyclus simulation after 2000 can be attributed to the real

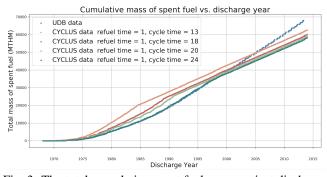


Fig. 3: The total cumulative spent fuel mass against discharge time for CYCLUS and UDB data from 1967 to 2013 for various cycle times.

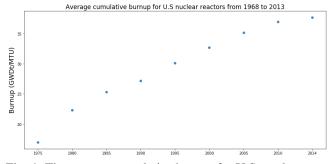


Fig. 4: The average cumulative burnup for U.S. nuclear reactors from 1968 to 2013 [16].

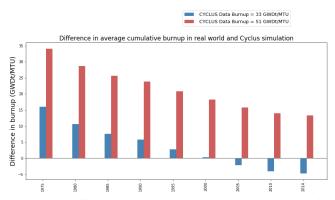


Fig. 5: The difference between average cumulative burnup for U.S. nuclear reactors and burnup used in Cyclus simulations.

world cycle lengths being shorter than the 18 month length of CYCLUS simulations. The United States DOE reported that there was a downward trend of forced outage rates of nuclear reactors from 2000 to 2014. The forced outage rate was 4.24% in 2000 and 2.98% in 2013 [15]. As the rate of forced outages decreased from 2000 to 2013, the cycle length also decreased.

Figure 3 includes plots of total spent fuel mass from Cxclus simulations where cycle time is varied. A shorter cycle time brings the total spent fuel mass from Cyclus simulations closer to the UDB data after 2000.

## Major Isotopic Composition of Spent Fuel Mass Comparison

To accurately simulate the U.S. nuclear fuel cycle from 1968 till the present, it important to use spent fuel recipes that have similar burnup in relation to the U.S. nuclear reactor burnup.

Figure 4 shows the average cumulative burnup for U.S. nuclear reactors from 1968 to 2013 [16]. Figure 5 shows the difference between burner of the spent fuel recipes used in the Cyclus simulations and cumulative burnup of U.S. nuclear reactors as seen in figure 4. On average, spent fuel burnup of 33 GWDt/MTU is closer to the cumulative burnup of U.S. nuclear reactors than 51 GWDt/MTU.

Figures 6 and 7 show the cumulative spent fuel isotopic mass difference between UDB and Cyclus data in 5 year intervals for burnup of 51 GWDt/MTU and 33 GWDt/MTU correspondingly. The Cyclus data that had 33 GWDt/MTU



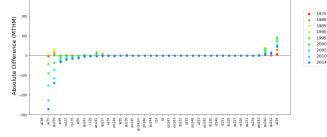


Fig. 6: The absolute difference between spent fuel mass from UDB data and CYCLUS data for each isotope for burnup of 51 GWDt/MTU (Positive difference means CYCLUS data is larger and negative difference means UP

Absolute difference between spent fuel mass from UDB data and CYCLUS data for each isotope for 33 GWDt/MTU

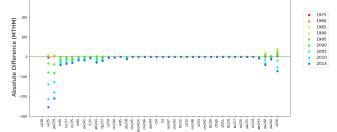


Fig. 7: The absolute difference between spent fuel mass from UDB data and Cyclus data for each isotope for burnup of 33 GWDt/MTU (Positive difference means Cyclus data is larger and negative difference means UDB data is larger).

burnup deviated less compared to the CycLus data that had 51 GWDt/MTU burnup. This is apparent for <sup>236</sup>U, <sup>242</sup>Pu and <sup>240</sup>Pu. They are similar for the isotopes on the left side of both figures. With an exception of <sup>239</sup>Pu having a substantial larger difference for 33 GWDt/MTU than 51 GWDt/MTU.

The impact of burnup on isotopic composition can be seen more clearly by looking at the cumulative spent fuel isotopic mass difference between UDB and CYCLUS data for the year 2000 (figure 8). In figure 4, at year 2000, the cumulative average U.S. nuclear reactor burnup was very close to 33 GWDt/MTU. Therefore, the difference in burnup between the U.S. nuclear reactor burnup and CYCLUS data burnup was around 20 GWDt/MTU for 51 GWDt/MTU burnup and 0 GWDt/MTU for 33 GWDt/MTU burnup (as seen in figure 5).

As discussed by Wigeland et al [17], <sup>240</sup>Pu, <sup>239</sup>Pu and <sup>241</sup>Am are the most significant long-term decay heat contributors to each waste package. While, <sup>238</sup>Pu, <sup>244</sup>Cm, <sup>90</sup>Sr and <sup>137</sup>Cs are the most significant short term decay heat contributors [17] to each waste package.

In figure 8, the CycLus simulation that uses the 33 GWDt/MTU burnup recipe has a small mass difference between UDB and CycLus data for <sup>240</sup>Pu and <sup>241</sup>Am compared to 51 GWDt/MTU burnup. However, it has a substantial difference for <sup>239</sup>Pu. Figure 4 also shows small differences between UDB and CycLus data for <sup>238</sup>Pu, <sup>244</sup>Cm, <sup>90</sup>Sr and <sup>137</sup>Cs.

The large mass difference between UDB and Cyclus data (where UDB <sup>239</sup>Pu mass is larger than Cyclus <sup>239</sup>Pu mass)

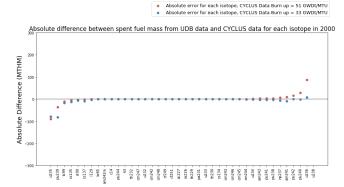


Fig. 8: The absolute difference between spent fuel mass from UDB data and CYCLUS data for each isotope at year 2000 for burnup of 33 GWd/MTU and 51 GWd/MTU (Positive difference means CYCLUS data is larger and negative difference means UDB data is larger).

for <sup>239</sup>Pu in figures 8, 6 and 7 can be attributed to conservative depletion parameters used in the calculations for isotopic compositions in the UDB database [7]. These assumptions result in the hardening of the neutron spectrum that results in increased <sup>239</sup>Pu production in the UDB data [7].

## CONCLUSIONS

This work demonstrates that the spent fuel mass and isotopic comparison results from the CYCLUS simulation of the United State huclear fuel cycle closely follow the results from real world metrics. This proves that these results can be used to produce accurate isotopic decay heat contributions and simulate loading of a waste repository based on thermal constraints. However, improvements can be made to more closely replicate reality.

Further work that would improve the simulation is to give the reactor age capability to accept varying cycle lengths, refueling times and spent fuel recipes. A Cyclus simulation then can be made to replicate the historic U.S nuclear fuel cycle even more closely by matching the cycle length, refueling time and specific reactors throughout their lifetime. This will give more accurate spent fuel mass and isotopic compositions which will in turn make the Cyclus simulations for loading of a waste repository more accurate.

#### ACKNOWLEDGMENTS

This research is being performed using funding received from the DOE Office of Nuclear Energy's Nuclear Energy University Program (Project 16-10512) "Demand-Driven Cycamore Archetypes". The authors want to thank members of the Advanced Reactors and Fuel Cycles research group (ARFC) at University of Illinois at Urbana Champaign in particular Jin Whan Bae for valuable advice and Gregory Westphal for proofreading. We also thank our colleagues from the Cyclus community, particularly those in the University of Wisconsin Computational Nuclear Engineering Research Group (CNERG) and the University of South Carolina Energy Research Group (ERGS) who provided collaborative support in the development of the core software, Cyclus, enabling this work.

# REFERENCES

- W. CARLSEN, M. GIDDEN, K. HUFF, 1. R. OPOTOWSKY, О. RAKHIMOV, A. С. A. M. SCOPATZ, Z. WELCH, and P. WIL-SON, "Cyclus v1.0.0," Figshare (Jun. 2014), http://dx.doi.org/10.6084/m9.figshare.1041745.
- 2. J. PETERSON, B. VAN DEN AKKER, R. CUM-BERLAND, P. MILLER, and K. BANERJEE, "UNF-ST&DARDS Unified Database and the Automatic Document Generator," Nuclear Technology, 199, 3, 310-319 (2017).
- 3. K. D. HUFF, M. J. GIDDEN, R. W. CARLSEN, R. R. FLANAGAN, M. B. MCGARRY, A. C. OPOTOWSKY, E. A. SCHNEIDER, A. M. SCOPATZ, and P. P. H. WIL-SON, "Fundamental concepts in the Cyclus nuclear fuel cycle simulation framework," Advances in Engineering Software, 94, 46-59 (Apr. 2016), arXiv: 1509.03604.
- 4. R. W. CARLSEN, M. GIDDEN, K. HUFF, A. C. OPO-TOWSKY, O. RAKHIMOV, A. M. SCOPATZ, and P. WILSON, "Cycamore v1.0.0," Figshare (Jun. 2014), http://figshare.com/articles/Cycamore\_v1\_0\_0/1041829.
- 5. K. D. HUFF, M. FRATONI, and H. R. GREENBERG, "Extensions to the cyclus ecosystem in support of marketdriven transition capability," Tech. rep., Lawrence Livermore National Laboratory (LLNL), Livermore, CA (2014).
- 6. M. BELL, "ORIGEN The ORNL Isotope Generation and Depletion Code," Tech. Rep. ORNL-4628, Oak Ridge National Laboratory (May 1973), software, Codes & Tools.
- 7. J. PETERSON, C. OLSON, J. ST. AUBIN, and B. CRAIG, "Additional Capability Being Developed from UNF-ST&DARDS Unified Database: System Analysis and Fuel Cycle Option Analysis," Nuclear Technology, 199, 3, 320-329 (Sep. 2017).
- 8. DOE, "Strategy for the Management and Disposal of Used Nuclear Fuel and High-Level Radioactive Waste," Tech. rep., United States Department of Energy, Washington D.C., United States (Jan. 2013).
- 9. IAEA, "PRIS Home," (2017).
- 10. P. WILSON, "The Adoption of Advanced Fuel Cycle Technology Under a Single Repository Policy," Tech. rep., University of Wisconsin - Madison (2009).
- 11. J. W. BAE, K. HUFF, and C. SINGER, "Synergistic Spent Nuclear Fuel Dynamics Within the European Union," in "Transactions of the American Nuclear Society Winter Conference," American Nuclear Society, Washington, D.C. (Oct. 2017).
- 12. RONACHER, "Welcome to Jinja2 âĂŤ Jinja2 Documentation (2.10)," (2018).
- 13. G. CHEE, G. T. PARK, and K. HUFF, "arfc/transitionscenarios : Validation of Spent Nuclear Fuel Output by Cyclus, a Fuel Cycle Simulator Code," (Jun. 2018).
- 14. IAEA, "Current Trends in Nuclear Fuel for Power Reactors," p. 11.
- 15. J. GEHIN, "Nuclear Power Reactors âĂŞ An Example of

Improvements in Reliability and Potential for Improvement," (Apr. 2016). 16. EIA, "Spent Nuclear Fuel," (Dec. 2015).

- 17. R. A. WIGELAND, T. H. BAUER, T. H. FANNING, and E. E. MORRIS, "Separations and Transmutation Criteria to Improve Utilization of a Geologic Repository," Nuclear Technology, 154, 95-106 (Apr. 2006).