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The Application of CYCLUS to Fuel Cycle Transition Analysis

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Abstract – *As part of the U.S. Department of Energy, Office of Nuclear Energy (DOE-NE) Fuel Cycle Options (FCO) campaign, a number of different software tools for computational nuclear fuel cycle simulation were used to model a transition scenario from the current to an advanced nuclear fuel cycle. A team of national laboratories conducted the modeling and analysis with different nuclear fuel cycle tools. Lawrence Livermore National Laboratory (LLNL), working with the University of California, Berkeley evaluated CYCLUS as part of this effort. CYCLUS is an agent-based fuel cycle simulator that uses discrete models representing the physics and behavior of nuclear fuel cycle processes (i.e. mining, fuel fabrication, chemical processing, transmutation, reprocessing, etc.). In this study, the capability of CYCLUS to perform a transition analysis is demonstrated, and plans for future code development to directly support the FCO effort are discussed.*

I. INTRODUCTION

As part of the U.S. Department of Energy, Office of Nuclear Energy (DOE-NE) Fuel Cycle Options (FCO) Campaign, an evaluation and screening (E&S) of potential nuclear fuel cycle options was performed, identifying a set of possible nuclear energy systems that meet certain performance and Research & Development (R&D) needs[1]. The next step in this FCO effort has been to analyze the features of a transition from the current nuclear fuel cycle in the United States to one of the future nuclear fuel cycles identified as "potentially promising", or having the potential to achieve the following performance benefits compared to the current U.S. fuel cycle with respect to the attributes specified in the E&S[1]:

- Greater than a factor of 10 reduction in the amount of high-level waste disposal.
- Greater than a factor of 1,000 reduction in the amount uranium disposal.
- Greater than a factor of 100 improvement in uranium utilization.

An FCO-led transition analysis (TA) effort has been established across several teams at national laboratories to model nuclear fuel cycle transition scenarios in the United States. Its objective is to explore how the nuclear fuel cycle in the U.S. can transition from the present once-through light water reactor (LWR) fuel cycle to an alternative fuel cycle implementing advanced reactor systems and nuclear technologies. The goals of the analysis are to understand the effects of different choices made during transition, to provide information on how transition may proceed, and how choices potentially made by decision makers could affect transition characteristics. Specifically, the transition analysis is meant to:

- develop a better understanding of transition issues (such as those involving timing, costs, associated obstacles, and others) in order to enable development of effective transition strategies,
- identify robust transition pathways that may be successful despite uncertainties related to technology advances, economic considerations, energy demand, etc., and
- identify the decisions that need to be made, the time frame for such decisions, and the effects of delaying decisions.[2]

The modeling and analysis was performed using the nuclear fuel cycle modeling codes VISION at Idaho National Laboratory (INL), ORION at Oak Ridge

National Laboratory (ORNL), DYMOND at Argonne National Laboratory (ANL), and CYCLUS at Lawrence Livermore National Laboratory (LLNL). Results were then compared across the tools.

CYCLUS was one of the codes used to support the broader FCO transition analysis effort. Lawrence Livermore National Laboratory (LLNL), working with the University of California, Berkeley and the University of Wisconsin-Madison, led this task. CYCLUS[3] is an agent-based fuel cycle simulator that uses discrete models representing the physics and behavior of nuclear fuel cycle components (i.e. mining, fuel fabrication, chemical processing, transmutation, reprocessing, etc.). To provide a starting point for users and developers, the CYCLUS team provides a suite of low-fidelity models within the Cycamore[4] project. Additionally, the design of CYCLUS allows custom capabilities, modules, and extensions to be developed by a user and developer community.

II. MODELS AND ASSUMPTIONS

II.A. Transition Analysis Base-Case Assumptions

As a result of the E&S effort, a comprehensive set of possible fuel cycles was assessed, but only several most promising potential future fuel cycles were identified. The transition from the current once-through nuclear fuel cycle (called “evaluation group 01” or “EG01”) to a fuel cycle implementing continuous recycle of uranium and plutonium with new natural uranium (NU) fuel in critical fast reactors (FR), also known as “evaluation group 23” or “EG23,” was identified as one of six scenarios of interest for the TA. The choice of EG23 was based on the lower barriers to entry in terms of development and deployment challenges that it offers compared to other promising fuel cycle options.

To have a basis of comparison across all fuel cycle simulators, all FCO teams evaluated the EG23 transition scenario using a common set of base-case parameters and assumptions. These include, but are not limited to:

- The transition timeline starts at 2015 and may run for 200 years (i.e. when the transition is complete and all LWRs have been replaced by fast reactors),
- 100 GWe of LWR installed capacity (operating at a 90% capacity factor) is online at the start of simulation and reactors are gradually decommissioned according to their assumed lifetime,
- 1% assumed annual growth rate in nuclear energy demand,
- Half of the legacy LWRs have 60-year lifetimes, and half have 80-year lifetimes,
- 40% thermal efficiency for fast reactors,
- Fast reactors are available for commercial deployment starting in 2050 and have 80-year lifetimes,
- New LWRs with 80-year lifetimes are constructed as needed before 2050, and fast reactors after that.
- Four nuclide tracking groups used for reactor mass balance calculations: uranium, plutonium, minor actinides, and fission products.

These base-case assumptions allowed each team to compare model results and evaluate each fuel cycle simulation tool in the context of the transition analysis.

II.B. Application of CYCLUS to the Transition Analysis

This analysis uses CYCLUS archetypes from three different sources. From the CYCLUS agents library, the Source, Sink, NullRegion, and NullInst archetypes were used. The Source and Sink facilities fill the same role as the corresponding structures in a system dynamics-based simulator. The Source is a generator of an exchangeable commodity, such as natural uranium. The Sink provides an end-of-life destination for resources and is used to represent the mass balance going to a deep geologic repository. The NullRegion and NullInst are a placeholder region and institution. Since the TA is only concerned about one region and looking at the entire fleet within that region, more sophisticated exchange behavior is not required by the specification.

From the Cycamore library, the simulation here only uses the DeployInst. This is an institution model whose role is to construct individual facilities at a predetermined time in the simulation. It is used here to build LWRs and FRs according to a preset deployment schedule. This is distinct from the NullInst, which here handles the facilities that always exist in the simulation such a reprocessing facilities and fuel fabrication facilities.

As an agent-based simulator, CYCLUS differs from many other dynamic fuel cycle simulators. The three most important distinctions are the implementation of a dynamic resource exchange solver (DRE) to construct a graph of all possible resource flows at each time step and solve this graph for a feasible exchange, a plug-in system for third-party models to be loaded into the simulation (alleviating the need for the models to be built into the simulator itself), and the ability to seamlessly handle many levels of model fidelity (known as multi-fidelity). However, the model implementations in Cycamore and

Bright-lite[5] are still under active development. This sacrifices short-term stability for long-term benefits. A significant portion of the ongoing development of Bright-lite and Cycamore is to support the requirements of the FCO-TA scenarios. Bright-lite, a medium-fidelity model, is currently under active development and has helped demonstrate the ability of CYCLUS to implement a third-party module. The reactor methodology of Bright-lite is distinct from lower-fidelity recipes-based models in that it is able to account for transient fuel composition behavior over the entire fuel cycle, even in non-equilibrium, full recycle scenarios. However, because Bright-lite is still under development, the results shown in this paper focus on the implementation of a low-fidelity model from Cycamore.

Driving deployment and decommissioning of facilities based on availability of material in the market has been a key challenge. The development of an institution archetype to support market-driven building and decommissioning of transitioning technologies was attempted[6]. In the market-driven model, a power demand curve is set and the model determines when to deploy reactor and support facilities. This is distinct from the DeployInst, which has no notion of demand and only adheres to a concrete deployment schedule. However, a simulation demonstrating a full market-driven deployment has not yet been completed.

Thus, while explicit deployment and decommissioning is currently possible in CYCLUS, efforts to drive it by logic internal to the core resource exchange paradigm have met algorithmic challenges requiring extra effort. Issues have also been identified with the resource exchange paradigm of the CYCLUS code. Additional debugging of the new archetypes and their interaction with the CYCLUS resource exchange paradigm remains as part of a future effort.[6]

Despite these challenges, it has been possible to meet transition analysis needs by implementing a pre-existing deployment schedule based on the solution of the DYMOND analysis (performed by ANL with DYMOND version 4.1.2)[7]. Using this deployment schedule to force new reactors to go online when they are needed, it was possible to model the transition from EG01 to EG23 with CYCLUS version 1.3.

The approach to modeling the transition analysis can be broken down into multiple stages of complexity. These stages reflect the needs of the TA effort at different levels. In the first stage of the effort, the capability of CYCLUS to perform the transition analysis was demonstrated. In this initial stage, and in order to demonstrate value in the fastest possible time frame, the support facilities were modeled as a fleet of facilities with an infinite capacity. In the CYCLUS simulation, this took the form of a single representative source agent. The deployed capacity available can be backed out as the amount of the material traded. The number of facilities that comprise the fleet is computable by dividing this capacity by the unit capacity given in the specifications for the baseline TA assumptions.

This strategy is for convenience and expediency, requires no additional archetype development effort, and allows the TA effort to focus on the short-term analysis needs. The assumption of infinite capacity of supporting facilities was considered to be reasonable for the initial analysis that could be used to determine the actual facility usage in the analysis. Those initial results could then be used in the follow-on analyses to size the facilities appropriately.

The Cymetric fuel cycle metrics calculator[8] was recently developed to facilitate access to a set of metrics that could be relevant to users of CYCLUS. Cymetric operates by reading data from a CYCLUS database, computing metrics (such as the total electricity produced), and writing those metrics back to the database. Previously computed metrics are stored for later retrieval and easy access.

In lieu of having an *in situ* market-driven deployment calculation, a post-processing wrapper was used to perturb the DYMOND deployment schedule, which can be seen in Appendix 1. Simulations with these perturbed schedules were then measured and ranked according to how well they fit the 1% growth rate target. The deployment schedule with the closest generated power to the target curve may then be selected as a “more fit” deployment schedule. The purpose of such an exercise is not to perform a multivariate optimization on the full fuel cycle EG01 to EG23 transition scenario. Rather, this is only to demonstrate that external wrapping of the Cyclus stack and evaluation of a cost function is possible and useful. Traditional optimization work is being pursued by others at UW and INL.

The DYMOND deployment schedule is given on an annual basis for the 200 year duration of the simulation. The simple perturbation study specifies four cases for each time step: increase the number of LWRs deployed by 1, decrease the number of LWRs deployed by 1 (minimum 0), increase the number of FRs deployed by 1, decrease the number of FRs deployed by 1 (minimum 0). Only a single time step is varied in any simulation. This generates a grid of 800 simulations (200 time steps times 4 cases per time step). This grid is small enough to execute explicitly on a single processor.

The objective function that was used is the sum of the absolute value of the difference between the total computed power and the 1% power demand curve, which starts at 90 GWe. For t being the time since the beginning of the simulation, x_t the total computed power [GWe] at time t, and then the objective $o(x)$ is given as:

$$o(x) = \sum_{t=0}^{200} |x_t - 90(1 + 0.01)^t|$$

The goal for the simple perturbation study is to find the deployment schedule that minimizes $o(x)$.

III. RESULTS AND DISCUSSION

Preliminary results discussed in this section demonstrate the capability of CYCLUS to model a nuclear fuel cycle transition scenario from EG01 to EG23. The base case simulation input file may be found in Reference 9.

The example scenario shown below uses a fixed reactor deployment schedule taken from a DYMOND-generated deployment schedule according to the EG23 transition scenario specifications[2]. This scenario assumes a staggered deployment of LWRs at a rate of 2 reactors per year from 1965 to 2015, to simulate a more realistic approximation of legacy LWR retirement profile during the transition window. The following results span a timeline of 250 years. The assumptions are those of the most recently discussed base-case scenario as described above. Infinite capacity of reprocessing facilities is assumed at the moment.

The reactor models implemented are fast burners (as opposed to breeders), represented by the Bright-lite reactor archetype[5]. This reactor model uses the full isotopic composition of the fuel and does not lump into U, Pu, MA, FP groups as specified by the base-case assumptions.

The following figures were generated via the Cymetric fuel cycle metrics calculator for the base case simulation.

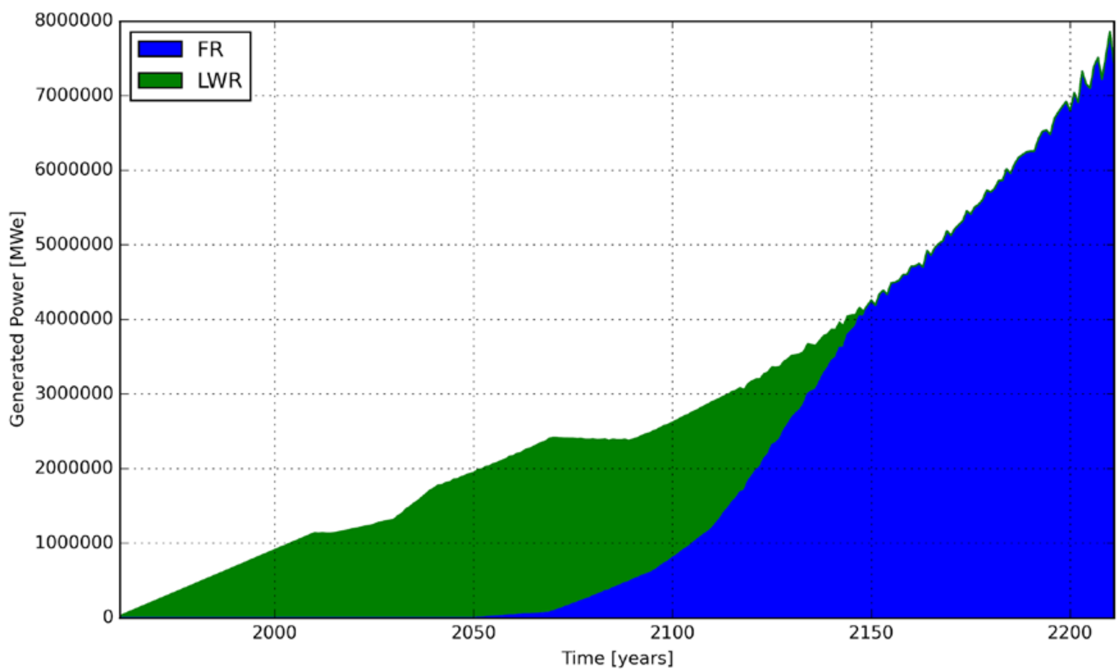

Figure 1: Total generated power, by reactor type.

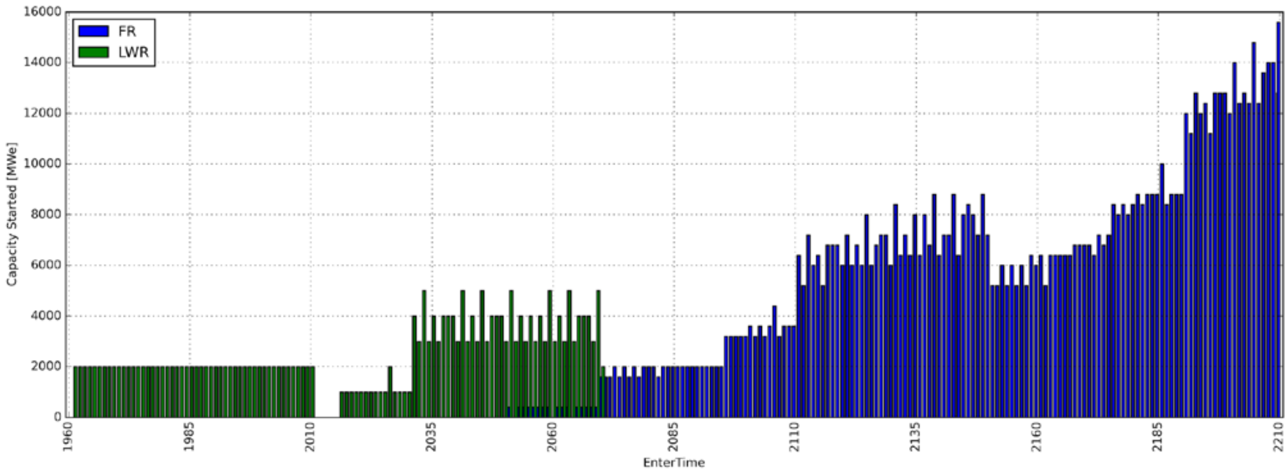

Figure 2: Reactor capacity deployed each year, by reactor type.

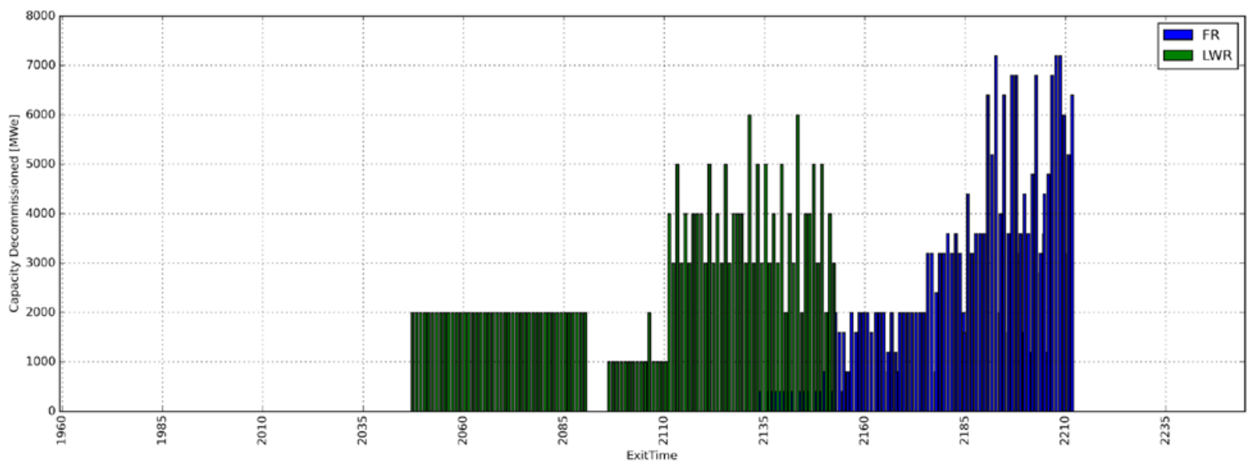

Figure 3: Reactor capacity retired each year, by reactor type.

Figures 1 - 3 match qualitatively with the same graphs generated by the DYMOND simulations from ANL. Given the large differences in modeling strategies between DYMOND and Cyclus, the agreement here is taken as a positive sign for the current capabilities of Cyclus. Furthermore, as expected, Figure 1 demonstrates exponential growth in the total power produced.

However, the facility deployment schedule could be modified to match a 1% power growth curve more precisely. This is the purpose of performing a preliminary searching study, as discussed at the end of Section II. The full suite of 800 perturbations was run and evaluated on the basis of the above objective function. From this study it was found that removing one fast reactor from the 8 that are deployed in year 2099 (time step t = 189) and instead only deploying 7 FRs yielded a total capacity curve that is closest to the 1% growth curve. This indicates that the deployment curve is overproducing power at this time.

The objective function value for the base case simulation is 642130.4 GWe using exactly the DYMOND deployment schedule. Meanwhile, the objective function value for the removal of one FR case as described above is 639542.4 GWe. This represents an improvement of 0.403% overall. Changing the deployment schedule by one reactor at one point in time does not significantly improve the total generated power. It is possible that more extensive changes to the schedule could yield even lower objective values. However, this preliminary study shows that CYCLUS can be used as the underlying engine to compute or modify facility deployment schedules.

IV. FUTURE WORK

In the next stages of the transition analysis using CYCLUS, the implementation of a deployment schedule for individual supporting facilities is planned, moving away from the fleet-based assumption of the model. This model will then be wrapped by an optimizer to determine a feasible deployment schedule. This shall prevent reactor deployment from being constrained by the support facilities.

CYCLUS has the potential to make supporting facility deployment based on the market utilization of the current facilities. This is known as the market-driven model described above. Ultimately, this functionality of CYCLUS is the most sophisticated and novel option and requires significant archetype and analysis capability development.

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APPENDIX I. Deployment Schedule

The following table is the deployment schedule that was used for the benchmark simulation and is what was perturbed during the preliminary search study.

TABLE I. Base Deployment Schedule for LWRs and FRs

Year	LWRs Deployed	FRs Deployed
2010	0	0
2011	0	0
2012	0	0
2013	0	0
2014	0	0
2015	1	0
2016	1	0
2017	1	0
2018	1	0
2019	1	0
2020	1	0
2021	1	0
2022	1	0
2023	1	0
2024	1	0
2025	2	0
2026	1	0
2027	1	0
2028	1	0
2029	1	0
2030	4	0
2031	3	0
2032	5	0
2033	3	0
2034	4	0
2035	3	0
2036	4	0
2037	4	0
2038	4	0
2039	3	0
2040	5	0
2041	3	0
2042	4	0
2043	3	0
2044	5	0
2045	3	0
2046	4	0
2047	4	0
2048	4	0
2049	3	0
2050	5	1
2051	3	0
2052	4	1
2053	3	1
2054	4	1
2055	3	1
2056	4	1
2057	3	1
2058	5	1
2059	3	0
2060	4	1
2061	3	1
2062	5	1
2063	3	0
2064	4	1
2065	4	1
2066	4	1
2067	3	1
2068	5	1
2069	2	4
2070	0	4
2071	0	4
2072	0	5
2073	0	4
2074	0	5
2075	0	4
2076	0	5
2077	0	4
2078	0	5

2079	0	5
2080	0	5
2081	0	4
2082	0	5
2083	0	5
2084	0	5
2085	0	5
2086	0	5
2087	0	5
2088	0	6
2089	0	5
2090	0	5
2091	0	5
2092	0	6
2093	0	5
2094	0	6
2095	0	8
2096	0	8
2097	0	8
2098	0	8
2099	0	8
2100	0	9
2101	0	8
2102	0	9
2103	0	8
2104	0	9
2105	0	11
2106	0	8
2107	0	9
2108	0	9
2109	0	9
2110	0	16
2111	0	14
2112	0	19
2113	0	15
2114	0	16
2115	0	14
2116	0	17

2117	0	17
2118	0	17
2119	0	15
2120	0	19
2121	0	15
2122	0	17
2123	0	15
2124	0	20
2125	0	15
2126	0	17
2127	0	18
2128	0	18
2129	0	15
2130	0	21
2131	0	16
2132	0	19
2133	0	16
2134	0	20
2135	0	16
2136	0	20
2137	0	17
2138	0	22
2139	0	16
2140	0	19
2141	0	18
2142	0	22
2143	0	16
2144	0	20
2145	0	21
2146	0	20
2147	0	18
2148	0	22
2149	0	19
2150	0	13
2151	0	14
2152	0	15
2153	0	14
2154	0	15

2155	0	14
2156	0	15
2157	0	14
2158	0	16
2159	0	15
2160	0	16
2161	0	14
2162	0	16
2163	0	16
2164	0	16
2165	0	16
2166	0	16
2167	0	17
2168	0	17
2169	0	17
2170	0	17
2171	0	16
2172	0	18
2173	0	17
2174	0	18
2175	0	21
2176	0	20
2177	0	21
2178	0	20
2179	0	21
2180	0	22
2181	0	21
2182	0	22
2183	0	22
2184	0	22
2185	0	25
2186	0	21
2187	0	23
2188	0	23
2189	0	23
2190	0	30
2191	0	29
2192	0	33
2193	0	30
2194	0	31
2195	0	29
2196	0	32
2197	0	32
2198	0	33
2199	0	30
2200	0	35
2201	0	31
2202	0	33
2203	0	31
2204	0	37
2205	0	31
2206	0	34
2207	0	35
2208	0	35
2209	0	32
2210	0	39