Fuel cycle transition simulation capabilities in Cyclus

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October 19, 2018

Abstract

Recent interest in advanced reactors and the following need for techno-economic transitions has increased the demand for tools necessary to model complex nuclear fuel cycles (NFCs) and advanced reactor technologies. This thesis demonstrates the capability of Cyclus, the agent-based fuel cycle simulator, to model, simulate, and analyze real-life fuel cycle transition scenarios. I introduce new methods and tools that use various databases to model and simulate real-world nuclear fuel cycle transition scenarios involving advanced reactor technologies.

The development of the capability takes three steps: (1) benchmarking Cyclus to other nuclear fuel cycle simulators (NFC simulators); (2) developing new methods and tools necessary for modeling and simulating real-world fuel cycle transition scenarios; (3) simulation of both domestic and international nuclear technology transitions.

The methods and tools developed for such capabilities include: (1) modeling and simulating past and current nuclear fleets using historic nuclear reactor operations database; (2) modeling individual reactors and its operating history to calculate nuclear material inventory; (3) modeling Molten Salt Reactor (MSR) behavior in a large-scale fuel cycle simulation.

Benchmark work show that Cyclus results coincide with results from other NFC simulators with minor differences due to modeling reactor behavior. Additionally, this thesis demonstrates the Cyclus capability to effectively model and simulate real-life NFC transition scenarios that involve advanced reactor technologies such as MSRs.

Acknowledgments

I consider all my output as a result of me standing on the shoulder of giants. There have been multiple giants that were kind enough to lend me their shoulders. Notably, the tallest of all, my advisor and mentor Kathryn Huff, who patiently guided me from my academic infancy. Also, I owe the world to my parents and loving brother who brought me up with love from my actual infancy. I also thank the staff of Oak Ridge National Laboratory Joushua L. Peterson-Droogh, Eva Davidson, Ben Betzler and Andrew Worrall for their guidance over the summer.

I also cannot express enough gratitude to my friends and colleagues. My greatest assets and partners that I have had the privilege to cohabitate with, Daniel O'Grady and Steven Stemmley, who were the logical anchor in my life. Also, my colleagues Andrei Rykhlevskii, Gwendolyn Chee, Gregory Westphal, Gyu Tae Park, Sun Myung Park, and Anshuman Chuabe have been of great help. Last but not least I thank my long-time friends Jieon Kim, Eric Bae, Daniel Stewart, Corey Burden, Shane Riew, Steve Chung, my comrades from the 12DIV Engineering 3CO, Christine Song, Gyum Hurr and Jae Man Jung.

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Chapter 1

Introduction

The scope of this work includes development and demonstration of various methods and tools to leverage Cyclus' existing capabilities to model real-world fuel cycle transition scenarios.

1.1 Background and motivation

Increasing climate change concerns have directed attention to nuclear energy, which produces reliable base load energy with negligible CO_2 emission. To reduce CO_2 emissions, the world will have to reduce fossil fuel based power plants. Also, the energy demand is expected to increase (28% growth between 2015 and 2040 [1]). Given the two circumstances, nuclear power is expected to play a crucial role in the world energy portfolio.

However, concerns of the accumulating UNF inventory, safety of the current reactor fleet, and the availability of uranium resources create a negative public perception of nuclear energy and its sustainability.

This work will demonstrate the capability of a system-level analysis tool, Cyclus, which can model a more advanced NFC that possibly solves the three concerned mentioned above. The modeling capability will aid in planning a strategy for transitioning into an advanced fuel cycle.

1.1.1 The Nuclear Fuel Cycle

The nuclear fuel cycle is described as a set of facilities that interact with one another to either provide or consume fuel services [2]. The general goal of the cycle is to produce power economically, while minimizing waste and natural resource used. The discharge UNF from the reactors is eventually sent back to facilities for either recycling or disposal.

The fuel cycle evaluation and screening study was conducted by Wigeland et al. to identify potential fuel cycles and to categorize them into 'evaluation groups' [3]. Wigeland et al. identified 40 fuel cycle groups, categorized by the extent of recycling (no recycle, limited recycle, and continuous recycle), fuel composition (e.g. thorium-U233, uranium-plutonium), and the type of reactors (fast/thermal critical reactors, sub-critical Externally Driven Systems (EDS)).

Once-through fuel cycle

In a once-through cycle, nuclear fuel is used once and then sent to storage without further reprocessing [4]. This cycle is often called the open fuel cycle, and is the current cycle for most nations with nuclear energy (e.g. U.S., Korea, Finland, Sweden).

This fuel cycle begins with mining of uranium ore, which is extracted from the ground. The mined ore is milled to form yellowcake (U_3O_8). The yellowcake is then either converted to UF_6 and enriched, or converted to UO_2 directly. This is because some reactor designs (e.g. Canada Deuterium Uraniums (CANDUs) [5]) can operate with natural uranium, while others (e.g. LWRs) need higher-than-natural levels of uranium-235. The processed UO_2 is then fabricated to pellets and loaded into fuel assemblies.

Once the fuel is depleted in the reactor, it is put in on-site pools to cool down. After cooling, the UNF is stored in dry casks as interim storage, destined to be sent to a geologic repository for permanent disposal.

Closed Fuel Cycle

In a closed fuel cycle, the UNF is recycled to be reused in a nuclear reactor. Recycling is not adopted worldwide due to concerns of high cost and proliferation, but has two major benefits: increased fuel utilization and reduction of repository burden.

UNF discharged from a typical LWR has an approximate composition: 95% uranium, 0.9% plutonium, 0.1% minor actinides, and 4% fission products [6]. The uranium, plutonium, and the minor actinides have the capability to produce power through fission. Thus, every group except the fission products can be separated to create new fuel for other reactors.

Additionally, repository capacity is constrained mostly by decay heat load and radioactivity, meaning that removal of the high-activity isotopes leads to a more efficient utilization of the repository capacity. Short-lived fission products (e.g. cesium, strontium) contribute to a large heat load and radioactivity in the first 100 years of UNF disposal, and minor actinides (americium, plutonium), with their long half-lives, contribute to longer-term heat and radioactivity in the repository [7], as shown in figure 1.1.

There are two major reprocessing technologies: methods that use low-temperature chemical separation using organic solvents (e.g. PUREX [8]), and methods that use high-temperature molten salts and metals, like pyroprocessing [9]. These methods separate the UNF into different streams, which are then sent to either a high level waste (HLW) repository (fission products) or an appropriate fuel fabrication facility (plutonium).

Different closed fuel cycles use different elemental groups for recycled fuel fabrication. For example, the PUREX process is used in La Hague in France [10], THORP in the U.K [11], Mayak in Russia, and Rokkasho in Japan to separated plutonium

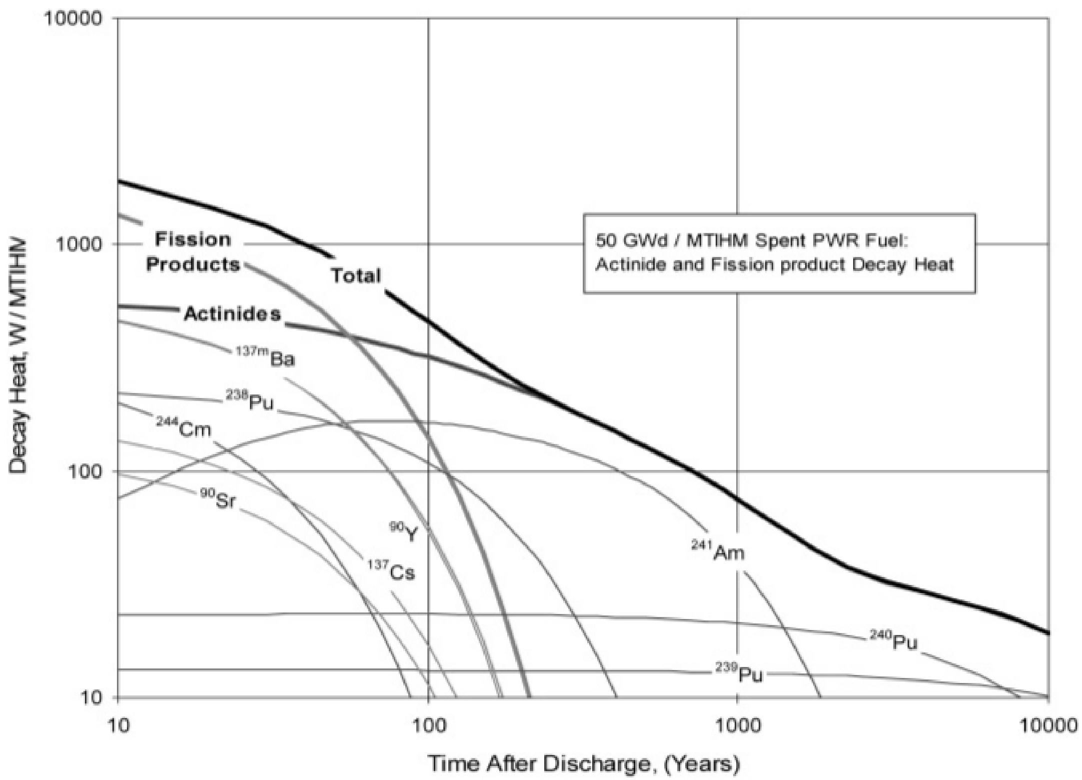

Figure 1.1: Decay heat contributions in UNF from a PWR irradiated to 50 GWd/MTHM. Reproduced from Wigeland, 2006 [7].

and uranium [12]. The plutonium is mixed with either depleted uranium (tails) or reprocessed uranium to produce Mixed Oxide Fuel (MOX).

Closed fuel cycles generally involve fast-spectrum reactors to control TRU inventory. A fast-spectrum reactor can be designed to either burn (reduce TRU), breed (produce more TRU), or break-even (maintain TRU amount). Selection of the fast-spectrum reactor design depends on the goal of the deploying institution.

In this work, I only transition into fuel cycles with continuous recycle of U/Pu or U/TRU with U fuel in fast critical reactors (Evaluation Group 23 or 24 from the Evaluation and Screening study[3]).

1.1.2 Fuel Cycle Transition Scenarios

Fuel cycle transition scenarios, in this work, are when once-through fuel cycles transition to closed fuel cycles through the progressive replacement of previous technology (e.g. LWR) with an advanced technology (e.g. reprocessing and fast-spectrum reactors). Analysis of transition scenarios requires deliberate tracking of materials and facilities in order to accurately calculate the resources necessary for a successful transition.

The timescale and feasibility of a transition scenario varies by nation, depending on the nation's nuclear energy demand growth, fuel cycle strategies, and initial conditions. In this work, I only consider the material feasibility of the transition scenario. Economic and political feasibility analyses are out of the scope of this work. A fuel cycle is is considered materially feasible if all the deployed reactors receive fuel in time.

The fuel demand is determined by two factors - nuclear energy demand growth and the nation's fuel cycle strategy. The nuclear energy demand growth determines the construction and operation schedule of new reactors, thus the expected fuel demand. Fuel cycle strategies determine the isotopic requirement of the fuel cycle transition scenario. For example, if the transition drives toward a U-Pu MOX fuel cycle, plutonium inventory dominates the timescale and feasibility of transition.

Once the expected fuel demand is calculated, the initial condition - current fissile material inventory and reactors (and their remaining lifetimes) - determines the material feasibility and timescale of a transition scenario. If a transition scenario is infeasible (i.e. fissile source is lacking), the transition can be 'loosened', by delaying deployment of advanced reactors. The energy demand is instead met by additional deployment of previous reactor technology (e.g. LWRs), thereby increasing transition timescale but reducing the intensity of fissile material demand.

Determining material feasibility of a NFC transition scenario requires dynamic tracking of material flows from multiple facilities, as well as modeling of complex systems. This work determines material feasibility by calculating the material inventory of real-world NFC transition scenarios.

1.2 Objectives

This thesis demonstrates and extends the real-world NFC transition scenario modeling capabilities in Cyclus. The goal is to develop tools that leverage Cyclus' modularity to add capabilities required for modeling real-world fuel cycle transition scenarios, and demonstrate Cyclus' capabilities by using the developed tools to perform NFC transition scenarios relevant to France and the United States.

1.3 Methods

This thesis accomplishes the objective in three steps. First, a benchmark showed good agreement with other fuel cycle simulation tools. [1] Second, I identified and developed the tools and methods necessary for modeling and simulating real-world transition scenarios. Finally, I constructed and ran fuel cycle transition scenarios relevant to France and the United States.

A previous study by Feng et al. [13] validates existing NFC simulators in a fuel cycle transition scenario, in which an LWR fleet transitions into an SFR fleet with continuous reprocessing. This study compares four well-known NFC simulators DYMOND [14], VISION [15], ORION [16], and MARKAL [17]. The results from each code were compared to a set of 'model solutions' that were generated from a spreadsheet for various metrics (e.g. fuel loading in reactor, UNF inventory). I reproduced the transition scenario in Cyclus, and compare the Cyclus results with those from the 'model solutions'.

In order to model real-world transition into an advanced fuel cycle, I developed two major tools. First, I developed `write_input.py` that automates extraction from the curated International Atomic Energy Agency (IAEA) Power Reactor Information System (PRIS) database [18]. The database lists each nuclear reactor's country, name, type, net capacity (Megawatt Electric (MWe)), status, operator, construction date, first criticality date, first grid date, commercial date, and shutdown date (if applicable). `write_input.py` extracts the information from this file to generate a Cyclus compatible input file, which lists the individual reactor units as agents. Second, I developed a module that models MSRs in Cyclus using a database generated from a high-fidelity MSR depletion calculation. The database is an output of Saltproc [??? Cite saltproc], a python module that drives SERPENT 2 [19] to model online reprocessing in an MSR. The database contains the historic compositions of each stream in and out of the reactor, composition history inside the reactor, and k_{eff} values. The developed tool then reads the database to mimic MSR behavior by requesting and offering feed and waste material to the Cyclus framework. The database is in HDF5 format, a hierarchical data format designed to store and organize large amounts of data [20].

Finally I constructed the fuel cycle transition scenario for France and the United States. I made different assumptions for the two scenarios to account for each nation's different goals, initial conditions (i.e. currently existing fleet, UNF inventory), and their potential reactor technology. I used the `write_input.py` to construct the initial

[1] These results have been submitted for publication in Annals of Nuclear Energy.

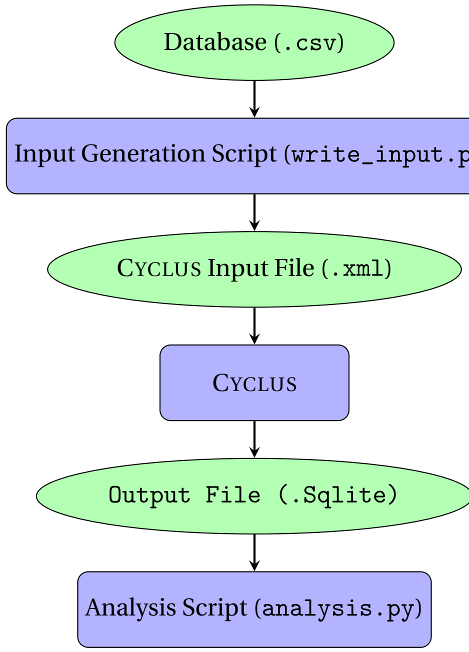

Figure 1.2: Green circles and blue boxes represent files and software processes, respectively, in the computational workflow.

Cyclus input file, followed by iterations to account for new reactor deployment. The workflow driving analyses is shown in diagram 1.2.

The structure of this thesis is as follows. In chapter 2, I review other fuel cycle simulation tools and their gaps, and explain the unique capability Cyclus has for transition scenario simulation. Chapter 3 explains the design and the development of capabilities needed for NFC transition simulation. Chapter 4 shows the results from the benchmark study, in which Cyclus results are compared to results from other fuel cycle simulation tools. Chapter 5 and 6 show the results from the France and United States fuel cycle transition scenario.

Chapter 2

Nuclear Fuel Cycle Simulators

NFC simulators are system-level analysis tools that allow tracking of material flow in a NFC. Their functionalities include, but are not limited to, isotopic decay, depletion calculations, and separation of material streams. The goal of a NFC simulator is to calculate *metrics* - quantitative measures of performance that can be compared among fuel cycle options [21].

The obtained metrics can then be optimized to the interests of different stakeholders. Passerini et al. [**?**] identified categories and criteria for NFC optimization and weighted the criteria for different stakeholders (e.g. Industry, laboratories). This approach can help decide which metric is important to stakeholders and optimize the fuel cycle for that metric.

Table 2.1 lists the NFC simulators considered in this section. The NFC simulators listed generally focus on one functionality (e.g. multi-regional analysis, detailed isotopic tracking, demand-driven deployment, cost analysis, sensitivity study) but lack in the flexibility to perform other functionalities [22]. In other words, no NFC simulator has all the functionalities to perform the superset of analysis types.

Table 2.1: List of NFC simulators considered in this paper. Reproduced from [22]

Name	Developer	Reference(s)
CAFCA	MIT	[23]
COSI6	CEA (Frane)	[24]
DANESS	ANL	[25]
DESAE2.1	Rosatom (Russia)	[26]
EVOLCODE2	CIEMAT (Spain)	[27]
FAMILY21	JAEA (Japan)	[28]
GENIUSv1	INL	[29]
GENIUSv2	Univ of Wisconsin	[30]
NFCSS	IAEA	[31]
NFCSim	LANL	[32]
VISION	ANL/INL	[15]

2.1 Capabilities required for modeling transition scenarios

A study by Brown et al. [33] identified nine common functionalities for NFC simulators for modeling transition scenarios - material compositions, deployment of fuel cycle facilities, front-end facility models, separations and material recycle facilities, reactor facilities, back-end features, starting the new fuel cycle, materials queuing and prioritization under capacity limitations, and energy demand algorithms. Brown et al. categorizes each functionality into three tiers - basic, integral, and exemplary. The functionalities, features, and their hierarchies are organized in table 2.2.

2.2 Additional capabilities identified for real-world fuel cycle transition scenarios

I identified three additional functionalities beyond the ones identified by Brown et al [33] for modeling real-world NFC transition scenario - integrating historical data, modeling discrete facilities and events, and modeling liquid-fueled reactors with continuous reprocessing.

2.2.1 Integrating historical data

In Modeling real-world nuclear fuel cycle transition scenarios, initial conditions (e.g. existing fissile inventory, existing reactor fleet) strongly impacts the transition scenario, such as reactor deployment schemes, fuel types, and reactor designs. This requires the NFC simulator to correctly model the current fleet and its remaining lifetime. The purpose of a fuel cycle is to produce power, thus the objective function of a fuel cycle simulation is generally to meet a certain power demand. Once the energy supply of the current fleet is calculated, the analyst can determine the deployment scheme of future reactors to meet a certain power demand in the future.

Past work on modeling real-world fleets

Modeling real-world fleets requires data about the current existing fleet, such as power capacity, core size, and expected shutdown date (remaining lifetime).

A study by Sunny et al. modeled the current U.S. nuclear fleet using ORION [34]. However, the fleet represented by Sunny et al. is far from modeling real-world U.S. nuclear fleet since it assumed an LWR deployed power capacity of 90 GWe in 2015, which decreases by 5 GWe every year starting from 2030, meaning that no consideration is given to the actual shutdown dates of existing reactors. This simplification stems from ORION modeling reactors as a fleet governed by a power demand, not discrete facilities.

Another study on the U.S. NFC transition scenario by Andrew Worrall [35] models actual U.S. nuclear fleets using the PRIS database, which is the same method used for this work. However, the analysis is done using an extensive network of spreadsheets, and not an NFC simulator.

Modeling real-world fleets is possible in Cyclus, for two reasons. First, Cyclus models discrete facilities with their own events and material flow. Second, Cyclus has a text-based input file structure, meaning that the input files (and thus the scenario) can be generated from a database and a script, as in this work.

2.2.2 Discrete reactor facility modeling

Discrete modeling of reactors allows a higher resolution of the power supply and material flow. In the real world, especially in the United States, existing reactors do not have the exact same power output or core size. This means that lumping the reactor fleet together causes a loss in accuracy. The loss in accuracy occurs by not capturing phenomena such as anisotropic fresh fuel fabrication requirements, spent fuel isotopics of a fleet of reactors with greatly varying burnups, and chaotic isotopic balance in fuel cycles involving multiple recycling passes [22]. NFC simulators like COSI 6 [24], EVOLCODE [27], FAMILY21 [28], do have discrete facility modeling capabilities, while DESAE2.2[26], and VISION [15] do not [36].

Similarly, most NFC simulators do not treat disruption events (lack of fuel supply, or decommissioning of a reactor) discretely. For example, ORION shuts down the entire simulation if there is a lack of fuel supply, and cannot decommission reactors mid-cycle. DESAE 'borrows' lacking fuel from storage (leaving a negative value) instead of shutting down the reactor [37]. COSI models reactors operating in sync [38].

2.2.3 Modeling liquid-fueled reactors with continuous reprocessing

MSR designs have recently gained attention due to their potential to be safer, more efficient, and sustainable [39]. Multiple companies in the U.S. are now pursuing commercialization of MSR design reactors, such as Transatomic [40] , Terrapower, Terrestrial [41], and Thorcon [42]. Other parties such as China (TMSR-LF [43]) , France (REBUS-3700 [44]), and the European Union (MSFR [45], MOSART [46]) are developing MSR designs.

However, modeling an MSR is challenging due to its online reprocessing and continuously flowing fuel. The material flow in and out of the reactor is continuous and dynamic, as well as the composition inside the core. The neutronics and depletion calculations have to be performed continuously while the composition of the fuel changes by depletion and reprocessing. Reactor physics and depletion calculations on the MSR have been done, notably by Oak Ridge National Laboratory researchers who developed ChemTriton [47], a python script that drives SCALE, to perform semi-continuous reprocessing of the fuel [48, 49]. However, no existing NFC simulator has the capability to model MSRs due to the large computational burden associated with frequent depletion calculations.

This challenge of large computational time in an NFC simulator can be overcome by 'outsourcing' the computationally heavy work to the higher-fidelity reactor physics and depletion codes. The output from the high-fidelity codes can be saved as a database, which then Cyclus reads to model the behavior corresponding to the MSR design. For example, a high-fidelity code would run a certain MSR design for its lifetime, and the history of its feed and waste recorded in a database. A Cyclus facility module would read this database and mimic the feed and removal behavior listed in the database, effectively modeling MSR interactions with the 'market'. This allows MSR modeling in a larger-scale system analysis without heavy computational burden, while securing fidelity of the depletion calculation.

Table 2.2: Nine common functionalities identified for NFC simulator to perform fuel cycle transition scenarios. Reproduced from Brown et al. [33]

Functionality	**Feature**	**Hierarchy**
Composition Features	Modeling of implicit consideration of fuel materials including primary fissile and fertile actinide isotopes	Basic
	Fuel's initial heavy metal mass modeled as lumped masses of the remaining actinides and fission products to conserve mass	Basic
	Isotopic decay of materials in storage	Exemplary
	Modeling of intermediate isotopes (e.g. Pa-233)	Exemplary
	Tracking of fission products beRyond a simple lumped sum	Exemplary
	Modeling of compounding materials in fuels and waste forms	Exemplary
Fuel Cycle Facility Deployment	Facility deployment and retirement	Basic
	Construction time delays	Basic
	Strategic deployment to meet demand	Integral
Front-end Facilities	Source (mining and milling)	Basic
	Details of mines and mills including annual and total quantities available	Exemplary
	Conversion and enrichment facilities	Basic
	Timing and capacity of recycle facilities	Basic
	Fuel fabrication	Basic
	Time delays and losses in separations and fabrication	Basic
Separations and Material Recycling	Separations facilities may be required for UNF	Basic
	Cooling time	Basic
	Losses in separations	Basic
	Material selection from the UNF supply	Basic
Reactor Facility	Fueling: number of batches, cycle length and fuel per batch	Basic
	Multiple fuel types in reactor facility (driver, blanket)	Basic
	Pre-generated charge and discharge isotopic compositions	Basic
	Real time calculations based on reactor physics models	Exemplary
	Reactor facility lifetime, construction time, and decommissioning time	Basic
	Initial charge for first core and discharge for final core	Basic
Back-end	Cooling of used fuel	Basic
	Conservation of mass - consistency with charged mass and generated power	Basic
Fuel Cycle Startup	External source of fissile material	Basic
	Startup on recycled fuel from other facilities	Integral
	Primary and back-up fuel types	Exemplary
Material Prioritization	Material accumulation	Basic
	Material prioritization	Integral
	Radioactive decay	Exemplary
Energy Demand Algorithm	Technology allocation accounting for availability	Integral
	Ordering and deployment of multiple reactor technologies	Integral

Chapter 3

Tools Used for this work

3.1 Cyclus

CYCLUS is an agent-based nuclear fuel cycle simulation framework [21], meaning that each reactor, reprocessing plant, and fuel fabrication plant is modeled as an agent. A CYCLUS simulation contains prototypes, which are fuel cycle facility models (archetypes) with pre-defined parameters, that are deployed in the simulation as `Facility` agents. Encapsulating the `Facility` agents are the `Institution` and `Region`. A `Region` agent holds a set of `Institutions`. An `Institution` agent can deploy or decommission `Facility` agents. The `Institution` agent is part of a `Region` agent, which can contain multiple `Institution` agents. Several versions of `Institution` and `Region` agents exist, varying in complexity and purpose [50]. `DeployInst`, which deploys agents at user-defined timesteps, serves as the `Institution` archetype in this work.

At each timestep, agents make requests for materials or bid to supply them and exchange with one another. A market-like mechanism called the dynamic resource exchange [2] governs the exchanges. For output analysis, each material resource has a quantity, composition, name, and a unique identifier.

In this work, each nation is represented as a distinct `Region` agent, that contains `Institution` agents, each deploying `Facility` agents. The `Institution` agents then deploy agents according to a user-defined deployment scheme.

The Cyclus NFC simulator framework and its modeling ecosystem, the suite of agents and other physics plug-in libraries compatible with it, incorporate modern insights from simulation science and software architecture [21]. Cyclus has multiple advantages over other available NFC simulators codes - open-source distribution, modularity, and extensibility. Its agent-based modeling approach is ideal for modeling coupled, physics dependent supply chain problems common in NFCs. The framework allows for dynamic loading of external libraries, which allows the users to plug-and-play different types of physics models for NFC simulation.

3.1.1 Open Source

License agreements and institutional approval are needed for most NFC simulators like COSI, DANESS, DESAE, EVOLCODE, FAMILY21, NFCSim, ORION and VISION [15], challenging both use and development in an academic setting. On the other hand, Cyclus relies completely on open source, free libraries, allowing all users to both use and develop the Cyclus framework and existing libraries. The open-source distribution of Cyclus encourages collaboration - any user can propose improvements or contribute extensions for Cyclus.

3.1.2 Modularity and Extensibility

In most modern NFC simulators, the facilities and their behaviors (and its fidelity) are confined in the software. Also, most modern NFC simulators model fuel cycles (once-through, continuous reprocessing) with immutable restrictions to connections between facilities. On the other hand, Cyclus allows users to plug-and-play various agent models within the Cyclus framework (shown in figure 3.1). Also, Cyclus relies on a market-based model for material trades between facilities, so the user can design any novel fuel cycle. This enables Cyclus to simulate any system analysis involving multiple connected facilities with physics-based calculations.

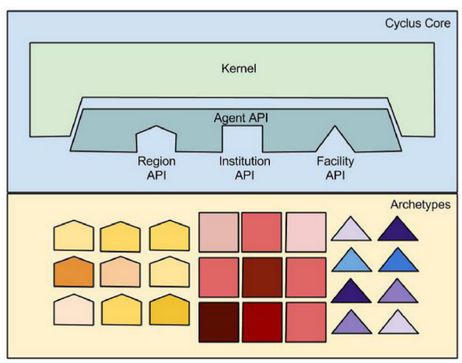

Figure 3.1: The Cyclus core provides APIs that the archetypes can be loaded into the simulation in a modular fashion [21].

Within the Cyclus kernel, the dynamic resource exchange (DRE) connects the framework and the agents by mediating agent material offers and requests. The kernel solves the multicommodity exchange problem posed by the material offers and requests and executes the transaction between two agents.

3.1.3 Cyclus' fitness for real-world NFC transition scenario

The Cyclus framework and its extension libraries fulfill all the functionalities specified by Brown et al. [33]. Additionally, its text-based input structure and discrete facility modeling capabilities allow modeling of real-world, individual reactors. Modularity in Cyclus enables adding an MSR model without altering Cyclus itself. The next chapter describes the MSR capability implementation in detail.

3.2 SaltProc

SaltProc is the on-line reprocessing simulation driver for SERPENT2 [51], for simulating liquid-fueled MSR operation [??? new zenodo]. SaltProc uses a semi-continuous approach to simulate continuous MSR material feed and removal [52]. It is coded in Python (compatible with both Python 2 and 3), and records feed, removal, and in-core isotopic history in an HDF5 [20] database.

SaltProc's structure and capabilities are similar to that of the ChemTriton tool for SCALE, developed at ORNL [53]. The computationally heavy work - Monte Carlo neutron transport and burnup calculations - are done in SERPENT, while SaltProc parses through the output material compositions, processes the fuel (removal and feed), and creates a new SERPENT input file. The user can specify removal rates, feed rates, and removal efficiencies for each isotope. At each timestep, the material compositions after the depletion calculation, and after fuel processing are recorded in the database, as well as the feed and removal stream.

The logical flow of SaltProc is illustrated in figure 3.2. Initially, SaltProc reads a user-defined SERPENT 2 input file that contains parameters such as geometry, non-fuel component composition, neutron population, criticality cycles, depletion time, total power, and boundary conditions. SERPENT 2 then performs neutron transport and depletion calculations and returns the number density of the depleted fuel. SaltProc then reads the depleted composition, writes the composition in the database, processes the depleted material according to a user-defined scheme, and then outputs a new fuel composition input card for SERPENT 2. This again is then read by SERPENT 2 and the cycle continues until the user-defined timestep is reached.

One of the benefits of having a semi-continuous external driver for SERPENT 2 is that the user can set up SaltProc so that the density of a certain isotope in the fuel remains constant. In other words, the feed rate can vary over time to meet a certain 'quality' of the fuel. Also, using a Monte Carlo code such as SEPRENT allows users to vary geometric fidelity, from a single cell model to a full core model.

3.2.1 Use in this work

SaltProc's output, the HDF5 database, can be imported through a Cyclus module that can mimic the MSR feed and removal behavior throughout its lifetime. The composition in the core can be ignored since the data of interest for a system-level NFC simulation is the material flow in and out of the reactor. This method can then effectively model MSRs in a large system-scale NFC simulation without a large computational burden for the NFC simulation.

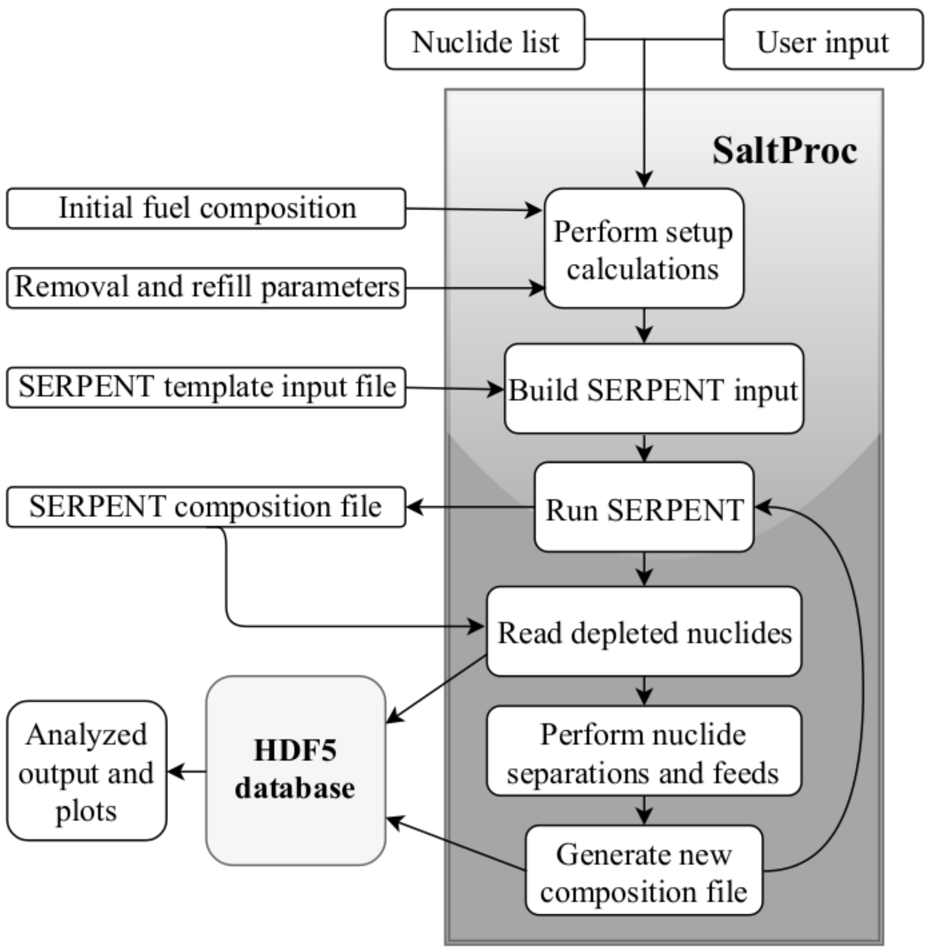

Figure 3.2: Flow chart for the SaltProc tool [52].

Chapter 4

Tools developed for this work

I developed two extensions to leverage the capabilities of Cyclus to model real-world fuel cycle transition scenarios. The first extension is a python input-generating module that automates scenario generation of the real-world nuclear fleet at any point in time. The second extension is a Cyclus archetype that mimics MSR feed and removal behavior using an HDF5 database generated from SaltProc.

4.1 write_input.py

The objective for `write_input.py` is to automate the generation of Cyclus input files to model the state of reactor fleets at a given point in time.

The module reads from the PRIS database [18] and extracts data on each reactor's country, reactor unit, type, net capacity (MWe), status, operator, construction date, first criticality date, first grid date, commercial date, and shutdown date (if applicable). The user inputs simulation configurations such as start year, start month, and simulation duration. The module uses the collected data to fill out a template into a Cyclus input file. The logical flow of the module is shown in diagram 4.1

4.1.1 Reactor deployment calculation

The module calculates the deployment scheme of reactors and their lifetimes by assuming that all reactors shut down after 60 years of operation. If the expected shutdown date is later than the user-input simulation start date, the reactor is not written in the input. If the reactor was operational prior to the simulation start date, and its shutdown date later than simulation start date, the reactor is deployed at the beginning of simulation with its remaining lifetime. If the reactor is reactor's start date is later than the simulation start date, and the shutdown time is undefined, the reactor is deployed at the defined start date with 60 years of lifetime.

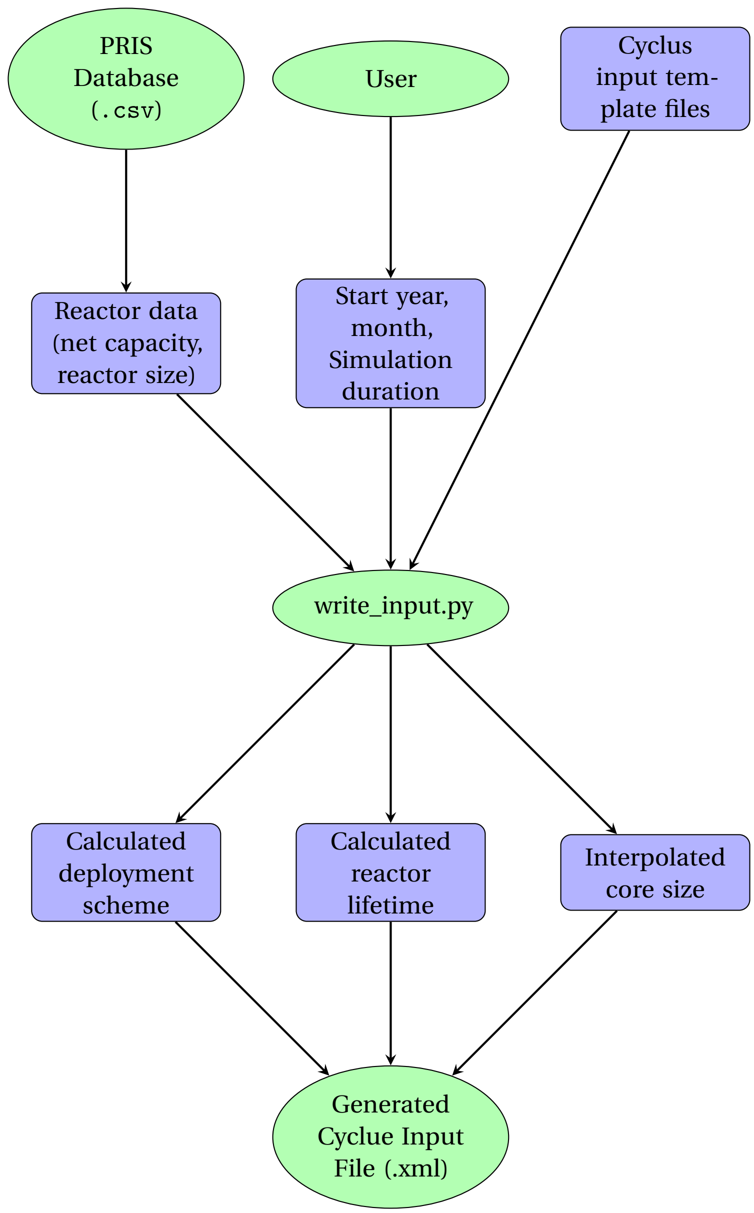

Figure 4.1: Logic flow of `write_input.py`. Green circles and blue boxes represent files and data, respectively.

4.1.2 Reactor parameter calculation

The module calculates the core sizes of various reactor types by using a linear core size model. It assumes that reactor cores scale linearly from a model reactor design, as shown in the equation below. The model reactor designs are listed in table 4.1.

$$N_{assem} = N_{assem.ref} * \frac{\mathrm{P}}{P_{ref}}$$

$$N_{assem.pwr} = 157 * \frac{\mathrm{P}}{1,100}$$

$$N_{assem.bwr} = 764 * \frac{\mathrm{P}}{10,098}$$

$$N_{assem.phwr} = 4,560 * \frac{\mathrm{P}}{700}$$

P = power capacity of reactor

Table 4.1: Reactor model designs used for the linear core size model.

Category	**Model Reactor**	**Power [MWe]**	**Assembly Mass [kg]**	**Assemblies in Core**	**Reference**
PWR	AP-1000	1110	446	157	[54]
BWR	4-MK I	1098	180	764	[55]
PHWR	CANDU6	700	24.17	4,560	[56]

4.2 HDF5-reactor

The HDF5 reactor is a Cyclus facility archetype designed to model MSR behavior using a database. It roughly couples “Saltproc” [52] and Cyclus, by using the output from SaltProc to mimic MSR feed and removal behavior in Cyclus. Most of the computationally heavy work (neutron transport calculations, fuel depletion calculation) is done in SERPENT (driven by Saltproc) in generating the database, which avoids the large computational burden when running Cyclus.

This method is similar to the simplified implementation of recipe reactors, where the depletion calculation is performed outside of the fuel cycle simulation. Instead of a single depletion calculation used in a recipe reactor, this reactor uses a database of recipes to capture the continuously varying nature of liquid-fueled reactors like MSRs.

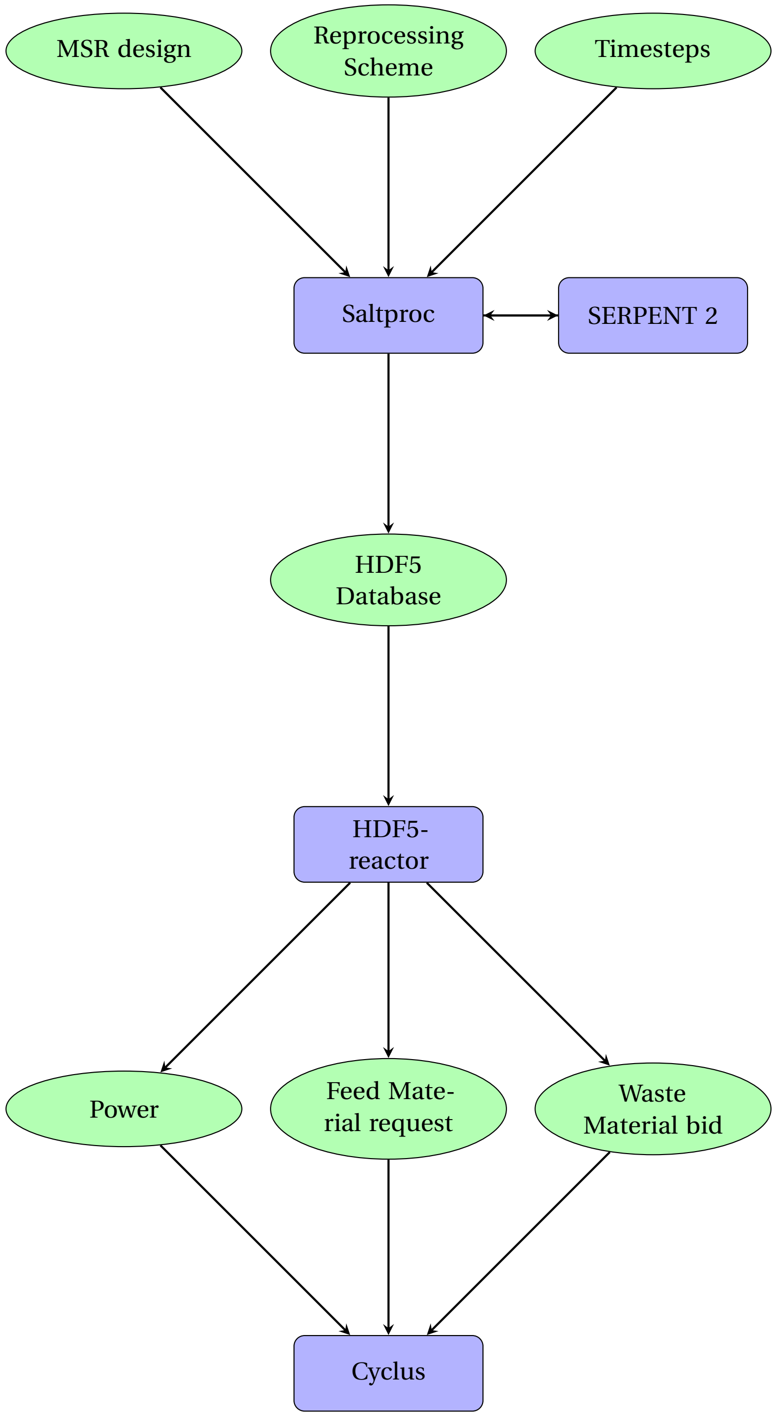

Figure 4.2: Logic flow of `HDF5 Reactor`. Green circles and blue boxes represent files and data, respectively.

4.2.1 Code Description

The user provides only of the commodity names for each stream (e.g. waste, fertile), and the database path, since the HDF5 database already contains the notion of reactor design, reprocessing scheme, and other reactor parameters (shown in figure 4.2). The commodity names are needed for reactor agents to communicate with other Cyclus agents in exchanging material.

At every timestep, The `HDF5 Reactor` calculates the material mass and composition accumulated during the Cyclus timestep, as shown in equation below.

$$M_T = \sum m_T$$

$$m_T = \sum_{t=(T-1)}^{T} m_t$$

M_T = total mass of stream in one Cyclus timestep

m_T = mass of isotope in one Cyclus timestep

m_t = mass of isotope in one Saltproc timestep

4.3 Limitations of the database approach

The limitations of this database approach is that it does not take into account the changing incoming fuel compositions due to decay. The separated TRU composition may vary depending on the time an LWR UNF has been cooled, thus affecting the performance of the MSR. The database approach assumes a fixed input salt composition, which is not the case in this simulation, because reprocessed TRU spends varying amounts of time until it is fabricated and put in the MSR.

This limitation is similar to that of batch-wise recipe reactors, where the pre-generated recipe already has a notion of the composition of initial fuel. This results in a depleted fuel composition that is agnostic to the incoming fuel composition in the simulation. For example, a batch-wise recipe reactor depleting a MOX fuel would depleted the MOX fuel to a same composition regardless of its plutonium vector. This is mediated by using fuel fabrication facility that modifies the plutonium enrichment to meet a certain fissile value (in Cyclus, the Cycamore `FuelFab` archetype).

The same method can be applied, where, instead of using a fixed mass ratio to fabricate fuel for MSRs, the fuel fabrication is done by modifying the TRU enrichment to match a certain fissile value. However, this is not a solution to solve the accuracy problem for depletion and errors in neutronics calculations.

Another way to overcome this limitation is to use a set of databases that contain multiple Saltproc simulation results with varying initial TRU vectors. When the reactor archetype receives the fuel, it will find the Saltproc simulation result with the initial fuel composition closest to that of the received fuel salt, minimizing error stemming from varying TRU compositions.

The best solution is to have a built-in depletion calculation model. However, as mentioned before, this requires too much computational burden for a fuel cycle simulation, where there are multiple reactors ‘at play’ at any given time. Another interesting method is to implement a reduced-order-model of MSR depletion behavior created by training from a large dataset of MSR simulations, such as Saltproc. This way, the computationally heavy work can be outsourced, and the variations in the initial fuel composition can be taken into account.

Chapter 5

Cyclus benchmark Study

This chapter demonstrates Cyclus' agreement with other NFC simulators by benchmarking the results of Cyclus to a previous verification study by Feng et al. [13]. This verification study compared four well-known NFC simulators DYMOND [14], VISION [15], ORION [16], and MARKAL [17]. The results from each code were compared to a set of 'model solutions' that were generated from a spreadsheet for various metrics (e.g. fuel loading in reactor, UNF inventory) in a transition scenario. I took the input parameters from this study, and reproduced the transition scenario in Cyclus, and compare the results. Results show that Cylcus' results are in good agreement with the results from Feng et al., with minor differences caused by reactor module behavior.

5.1 Methodology

Feng et al. comprehensively defines simulation parameters sufficient to reproduce the transition scenario in CYCLUS. In this study, we used the CYCAMORE [21] archetype library to model all fuel cycle facilities. CYCAMORE libraries are archetypes maintained by the core developer team.

CYCLUS results are output in either `.sqlite` or `.h5` format. In this study, we used the `.sqlite` format and analyzed the results using python. The post-processed output data was overlapped with the results with the model solution from the verification study [13]. The input file and analysis procedures are all available on Github [57].

5.2 Fundamental Modeling Differences in CYCLUS

CYCLUS has fundamental modeling choice differences from the fuel cycle analysis codes used in the benchmark [13].

CYCLUS has a default time step of a month. The verification study solutions are evaluated with 1-year time steps, so cumulative and annual averages were used. For example, decommissioning facilities occurs at the end of a timestep, and building facilities occurs at the beginning of a timestep.

The CYCAMORE recipe reactor depletes half of its core when decommissioned mid-cycle, whereas the codes in the benchmark [13] deplete all their reactors' fuel when decommissioned. For this study, we changed the CYCAMORE source code to deplete all its assemblies to the depleted recipe. Also, the CYCAMORE recipe reactor treats each batch (and assembly) as a discrete material, while some codes have continuous fuel discharge. This produces differences in the results because the batches in the benchmark [13] are in time-averaged values. In this study, the LWR batch size and cycle time is increased, while decreasing the batch number to keep the core size constant. We round up the SFR batch number, while the batch size and cycle time are kept constant. This increases the core size by 1.08%, which is negligible, but will be discussed in the results section. The differences are listed in table 5.1.

Table 5.1: Difference in Batch number and core size

Category	**Benchmark[13]**	**CYCLUS**
LWR Batches	4.5	3
LWR Batch size [tHM]	19.91	29.86
LWR Core size [tHM]	89.59	89.59
LWR Cycle time	1 year	1.5 years
SFR Batches	3.96	4
SFR Batch size [tHM]	3.95	3.95
SFR Core size [tHM]	15.63	15.8

Note that the Cyclus framework code would never need to be changed. However, the only change made was the reactor depletion behavior at decommission due to its large impact on plutonium inventory. The goal of this study is to show current CYCLUS agreement with other codes and identify differences, not to alter CYCLUS to match the other codes.

5.3 Results

We obtained the benchmark solutions through personal contact with benchmark author Bo Feng at Argonne National Laboratory.

Figure 5.1 shows the deployed reactor capacity, and figure 5.2 shows the LWR retirement and SFR deployment. The two plots show exact agreement with the benchmark solutions.

Figure 5.3 shows the annual fuel loading rate. The initial fuel loading for 100 LWR reactors are not shown in the plot for both the benchmark and the Cyclus results. The oscillations caused by the 18 month refueling period were aggregated into 12 month groups. As a result the total fuel loaded is equal for both plots.

Although indistinguishable in figure 5.3, there is a small difference between SFR fuel loading proportional to the core mass difference, because Cyclus only has integer batch numbers. Figure 5.4 shows the differences normalized by the core mass differences, overlapped with the SFR deployment. This shows that the differences only occur during deployment due to the difference in core mass.

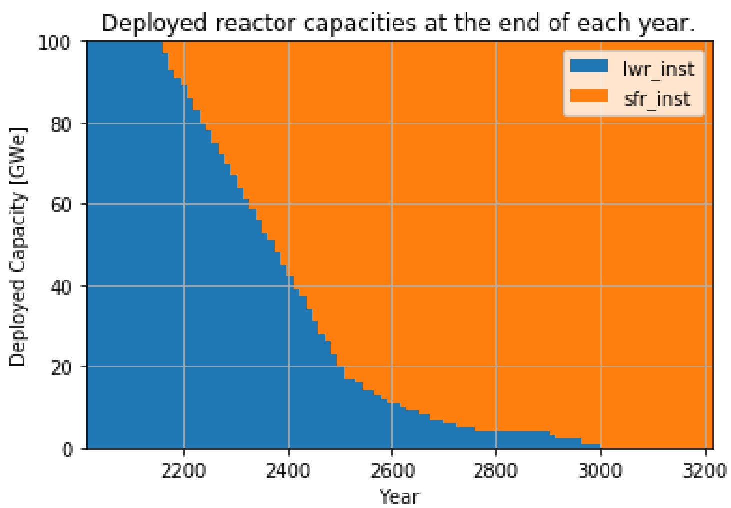

Figure 5.1: Deployed reactor capacities at the end of each year from Cyclus.

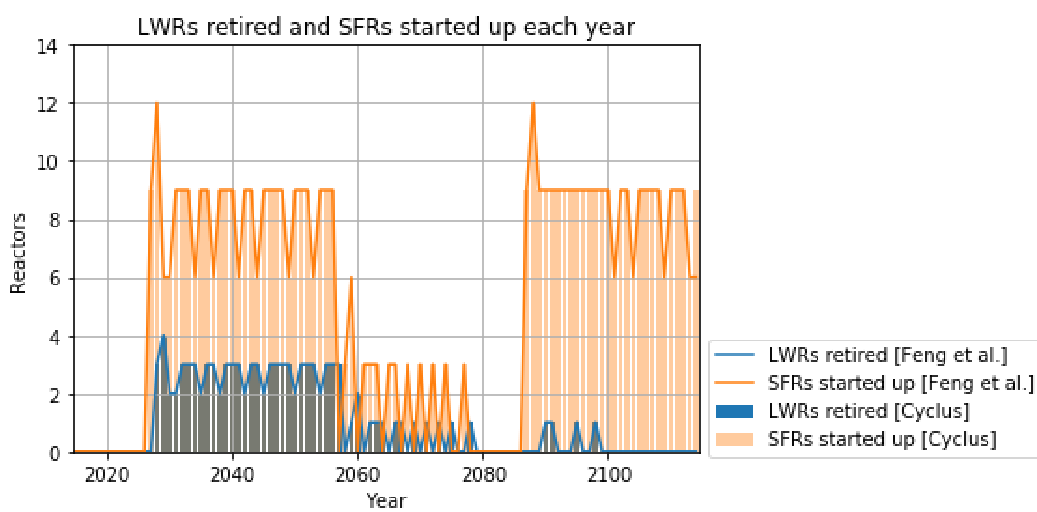

Figure 5.2: LWRs retired and SFRs started up each year.

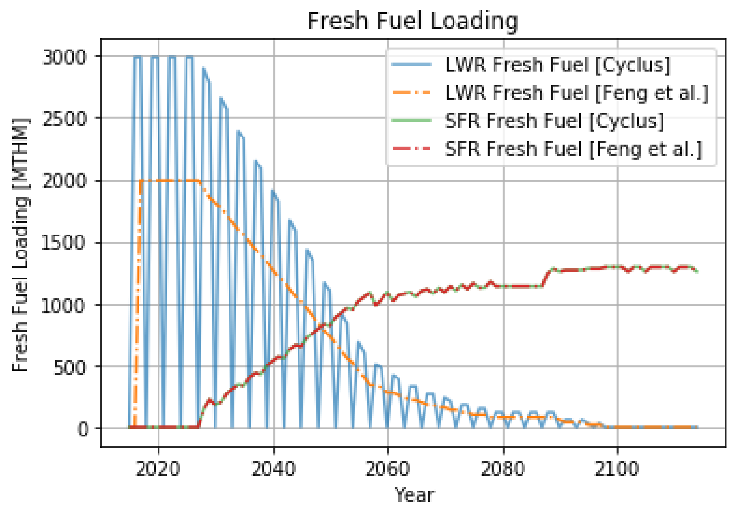

Figure 5.3: Annual fresh fuel loading rates (first cores and reload fuel).

Figure 5.5 shows the inventory of discharged UNF in the mandatory cooling stage (four years for LWR, one year for SFR). It also oscillates around the benchmark's solution and converges, due to the influx and the outflux of UNF into and out of the storage facility. The SFR inventory and fuel loading solutions exactly matches the benchmark solutions, minus the small (1.07%) difference due to core size.

Figure 5.6 shows the amount of cooled UNF waiting for reprocessing. The value is calculated by subtracting the cumulative difference between the cooled inventory and the UNF reprocessing throughput.

$$M_{wait,t} = M_{cooled,t} - M_{rep,t}$$

The oscillation is between the cooled inventory in the storage facility before (high) and after (low) it sends its inventory for reprocessing.

Figure 5.7 shows the reprocessing throughput, which oscillates around the benchmark solution. No oscillation exists from 2030 to 2055 because the LWR UNF reprocessing plant throughput peaks at 2,000 tons per year.

Figure 5.8 shows the inventory of unused TRU recovered from UNF. The CYCLUS results follow the benchmark solutions closely. However, the larger SFR core size in Cyclus causes CYCLUS results to be 1.07% smaller than the benchmark results, since more TRU is used to start up the newly deployed SFRs.

5.4 Discussion

We verified CYCLUS with results from an established verification study and saw good agreement in a transition scenario.

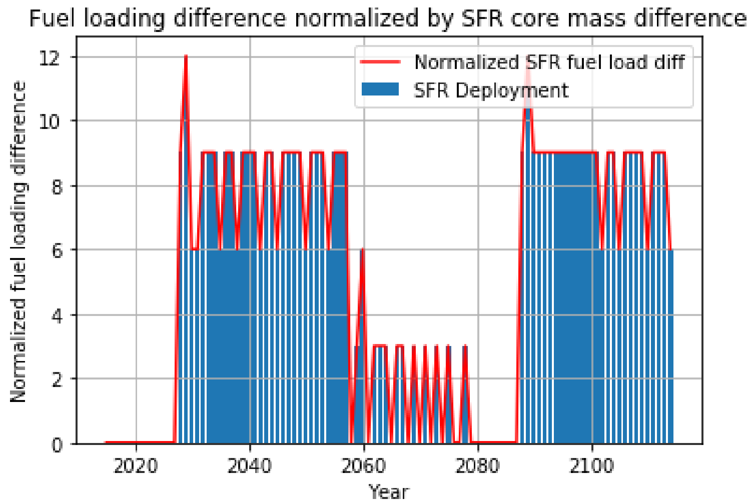

Figure 5.4: Difference between annual fresh SFR fuel loading rates (Cyclus - Benchmark) normalized by the core mass difference of an SFR due to fractional batch size.

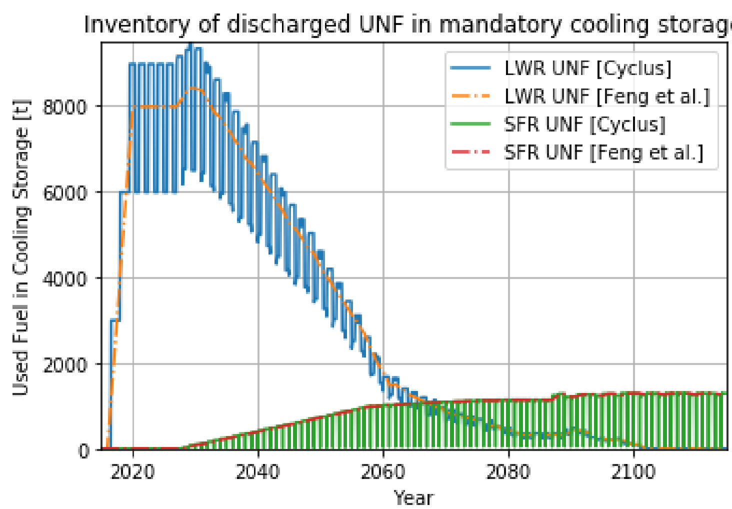

Figure 5.5: Inventory of discharged UNF in mandatory cooling storage.

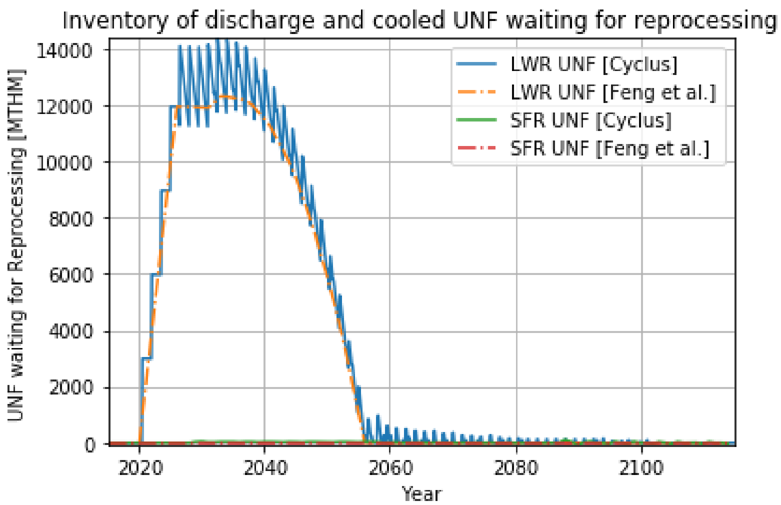

Figure 5.6: Inventory of discharged and cooled UNF waiting for reprocessing.

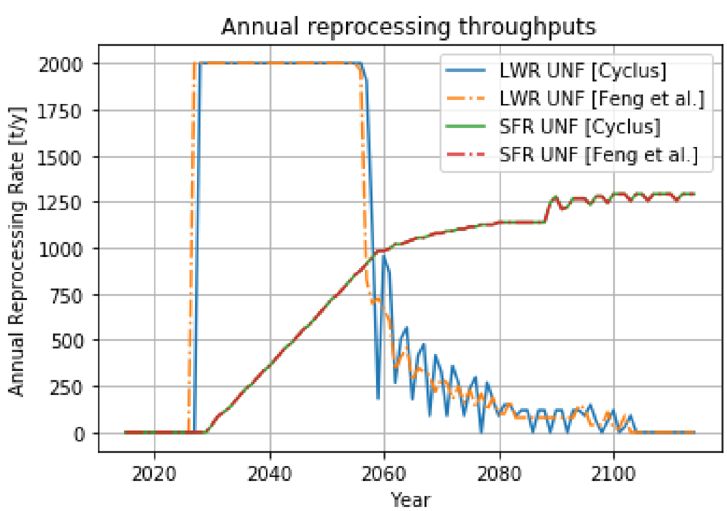

Figure 5.7: Annual reprocessing throughputs.

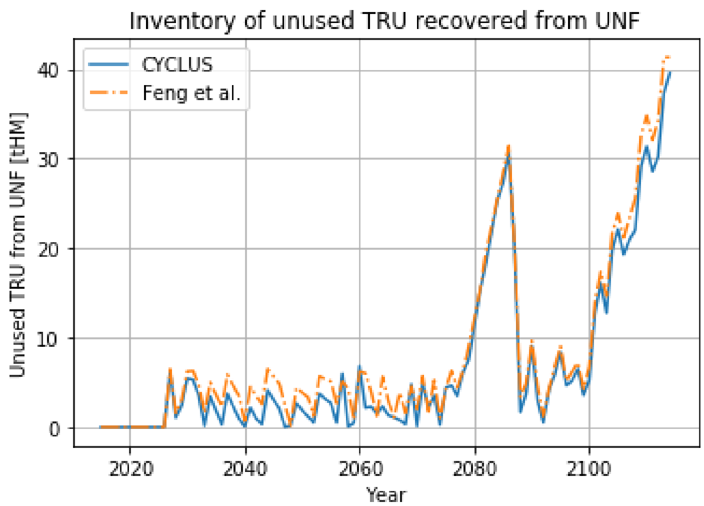

Figure 5.8: Inventory of unused TRU recovered from UNF.

Throughout this work, two major differences were identified that led to the deviation of CYCLUS results from that of the benchmark solution. First, the CYCAMORE reactor depletes only half of its core when decommissioned. Second, CYCLUS, unlike other codes examined in the benchmark (except ORION), fully resolves discrete batches for fuel discharge. We resolve the first discrepancy by changing one line in the Cycamore source code.

This study proves that CYCLUS is a capable tool for modeling fuel cycle transition scenarios.

Chapter 6

French NFC Transition Scenario with EU Regional Analysis

The stated long term plan for nuclear deployment in France targets a technology transition to SFRs [58]. However, the current inventory of French UNF is insufficient to fuel that transition without building new LWRs [59].

If instead, France accepted UNF from other EU nations and used it to produce MOX for new SFRs, the MOX created will fuel a French transition to an SFR fleet and allow France to avoid building additional LWRs.

To simulate this cooperative scenario, I simulated the entire EU region and all its nuclear reactor operating history and UNF accumulation up to the nearest foreseeable future. Then, France takes as much UNF it needs to transition into a fully SFR fleet without building additional LWRs.

This chapter includes the results from a French NFC transition scenario from a LWR fleet to a fully SFR fleet by taking other EU nations' UNF.

6.1 EU Deployment Schedule

The historic EU deployment schedule and operation history are generated using the `write_input.py` module (described in section 4.1).

Projections of future reactor deployment in this simulation are based on assessment of analyses from references, for instance PRIS, for reactors planned for construction [60], the World Nuclear Association [61], and literature concerning the future of nuclear power in a global [62] and European context [63]. Existing projections extend to 2050.

Table 6.1 lists the reactors that are currently planned or under construction in the EU. In the simulation, all planned constructions are completed without delay or failure and reach a lifetime of 60 years.

Table 6.1: Power reactors under construction and planned. Replicated from [61].

Exp. Operational	**Country**	**Reactor**	**Type**	**Gross MWe**
2018	Slovakia	Mochovce 3	PWR	440
2018	Slovakia	Mochovce 4	PWR	440
2018	France	Flamanville 3	PWR	1600
2018	Finland	Olkilouto 3	PWR	1720
2019	Romania	Cernavoda 3	PHWR	720
2020	Romania	Cernavoda 4	PHWR	720
2024	Finland	Hanhikivi	VVER1200	1200
2024	Hungary	Paks 5	VVER1200	1200
2025	Hungary	Paks 6	VVER1200	1200
2025	Bulgaria	Kozloduy 7	[1]AP1000	950
2026	UK	Hinkley Point C1	EPR	1670
2027	UK	Hinkley Point C2	EPR	1670
2029	Poland	Choczewo	N/A	3000
2035	Poland	N/A	N/A	3000
2035	Czech Rep	Dukovany 5	N/A	1200
2035	Czech Rep	Temelin 3	AP1000	1200
2040	Czech Rep	Temelin 4	AP1000	1200

For each EU nation, we categorize the growth trajectory from “Aggressive Growth” to “Aggressive Shutdown”. “Aggressive growth” is characterized by a rigorous expansion of nuclear power, while “Aggressive Shutdown” is characterized as a transition to rapidly de-nuclearize the nation’s electric grid. We categorize each nation’s growth trajectory into five degrees depending on G, the growth trajectory metric:

$$G = \left\{ \begin{array}{ll} \text{Aggressive Growth,} & \text{for } G \geq 2 \\ \text{Modest Growth,} & \text{for } 1.2 \leq G < 2 \\ \text{Maintanence,} & \text{for } 0.8 \leq G < 1.2 \\ \text{Modest Reduction,} & \text{for } 0.5 \leq G < 0.8 \\ \text{Aggressive Reduction,} & \text{for } G \leq 0.5 \end{array} \right\} = \frac{C_{2040}}{C_{2017}}$$

$$G = \text{Growth Trajectory } [-]$$

$$C_i = \text{Nuclear Capacity in Year i } [MWe].$$

The growth trajectory and specific plan of each nation in the EU is listed in Table 6.2.

[1]The fate of many planned reactors is uncertain. The proposed reactor types are also unclear. The ones marked ‘N/A’ for type are assumed to the PWRs in the simulation.

Table 6.2: Projected nuclear power strategies of EU nations [61]

Nation	Growth Trajectory	Specific Plan
UK	Aggressive Growth	13 units (17,900 MWe) by 2030.
Poland	Aggressive Growth	Additional 6,000 MWe by 2035.
Hungary	Aggressive Growth	Additional 2,400 MWe by 2025.
Finland	Modest Growth	Additional 2,920 MWe by 2024.
Slovakia	Modest Growth	Additional 942 MWe by 2025.
Bulgaria	Modest Growth	Additional 1,000 MWe by 2035.
Romania	Modest Growth	Additional 1,440 MWe by 2020.
Czech Rep.	Modest Growth	Additional 2,400 MWe by 2035.
France	Modest Reduction	No expansion or early shutdown.
Slovenia	Modest Reduction	No expansion or early shutdown.
Netherlands	Modest Reduction	No expansion or early shutdown.
Lithuania	Modest Reduction	No expansion or early shutdown.
Spain	Modest Reduction	No expansion or early shutdown.
Italy	Modest Reduction	No expansion or early shutdown.
Belgium	Aggressive Reduction	All shut down 2025.
Sweden	Aggressive Reduction	All shut down 2050.
Germany	Aggressive Reduction	All shut down by 2022.

Using this categorization to drive facility deployment, Cyclus captures regional differences in reactor power capacity and UNF production as a function of time. Accordingly, fig. 6.1 shows the resulting simulated installed capacity in EU nations. Sudden capacity reductions seen in the 2040s result from end-of-license reactor retirements and nuclear phaseout plans in nations such as Germany and Belgium.

6.2 French SFR Deployment Schedule

Figure 6.2 shows the French transition to SFRs modeled in this simulation. Historically aggressive growth of nuclear in the 1980s leads to a substantial shutdown of nuclear in the 2040s, which, in the simulation, are replaced by new SFRs. The net capacity is kept constant at 66 GWe.

Figure 6.3 shows the deployment strategy required to support the transition in fig. 6.2. France must build four reactors per year, on average, to make up for the end-of-license decommissioning of power plants built in the 1980s and 1990s. The second period of aggressive building occurs when the first generation of SFRs decommission after 80 years. Starting in 2040, France deploys 600-MWe SFRs to make up for decommissioned French LWR capacity. This results in an installed SFR capacity of 66,000 MWe by 2078 when the final LWR is decommissioned.

Finally, Figure 6.4 shows the total deployment scheme we simulated. The French transition to SFRs couples with the historical and projected operation of EU reactors. The steep transition from 2040 to 2060 reflects the scheduled decommissioning of reactors built in the 1975-2000 era of aggressive nuclear growth in France.

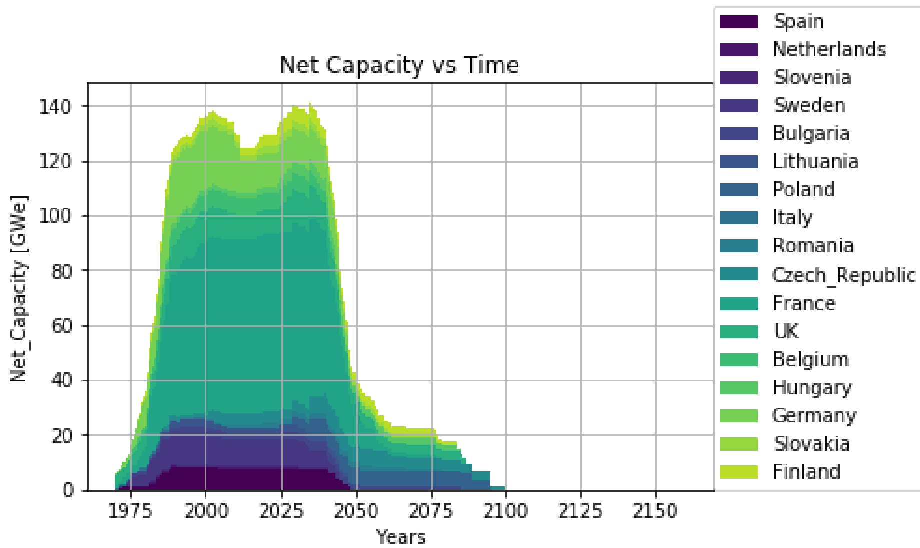

Figure 6.1: Installed nuclear capacity in the EU is distinguished by `Regions` in CYCLUS.

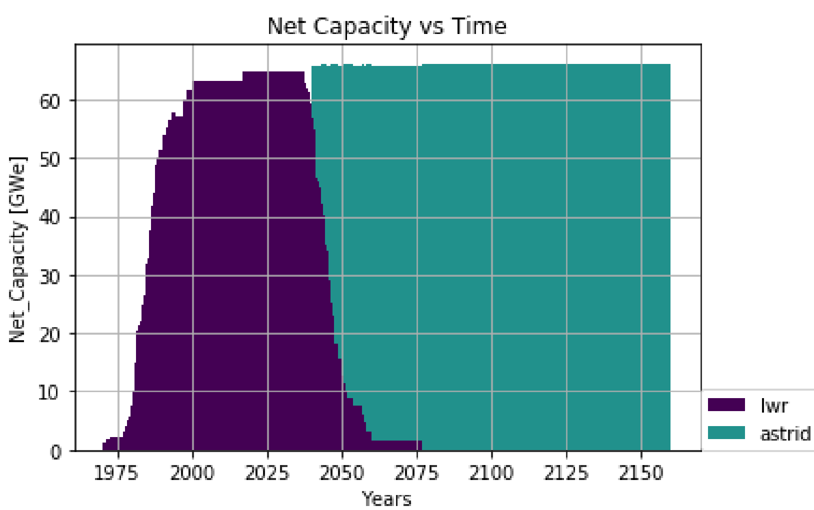

Figure 6.2: The potential French transition from LWRs to SFRs when assisted by UNF from other EU nations.

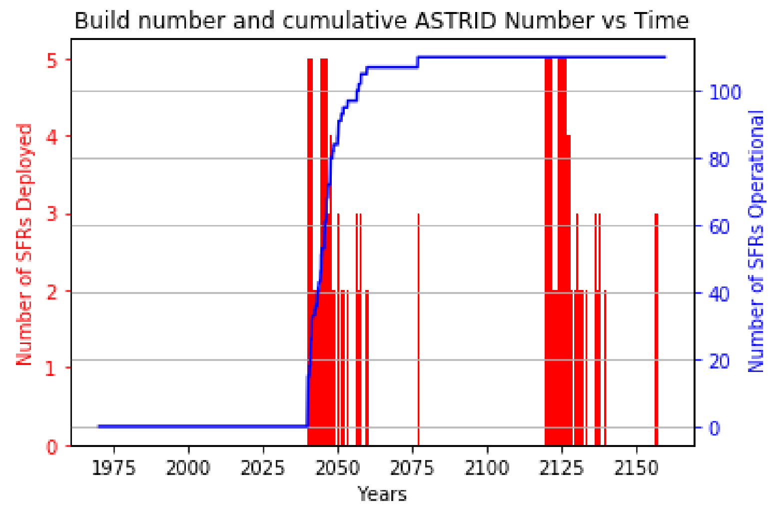

Figure 6.3: The simulated deployment of SFRs in France is characterized by a period of aggressive building.

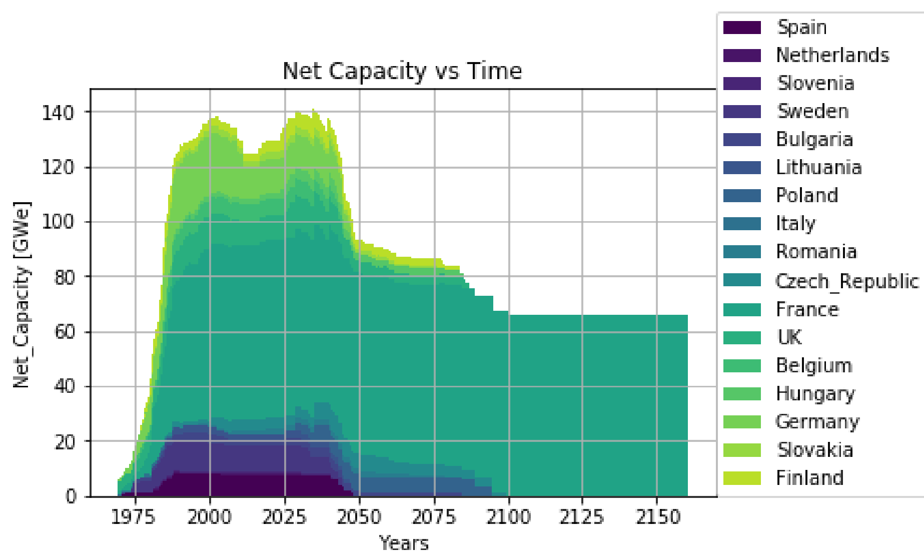

Figure 6.4: The total simulated deployment scheme relies on UNF collaboration among nations.

These figures reflect that, for the given assumptions, bursts of construction are necessary to maintain capacity. In reality, a construction rate of five reactors every year is ambitious, but might have the advantage of larger scale production of components and more modular assembly and construction if major components can mostly be built off site. I performed additional simulations assuming random LWR license extensions, to decrease the number of new reactor deployment.

This analysis establishes a multi-national material flow and demonstrates that, if such an aggressive deployment scheme took place, the SFRs would have enough fuel.

6.3 Material Flow

The fuel cycle is represented by a series of facility agents whose material flow is illustrated in figure 6.5, along with the CYCLUS archetypes that were used to model each facility. In this diagram, MOX Reactors include both French PWRs and SFRs.

A mine facility provides natural uranium, which is enriched by an enrichment facility to produce UOX. Enrichment wastes (tails) are disposed of to a sink facility representing ultimate disposal. The enriched UOX fuels the LWRs which in turn produce spent UOX. The used fuel is sent to a wet storage facility for a minimum of 72 months. [59].

The cooled fuel is then reprocessed to separate plutonium and uranium, or sent to the repository. The plutonium mixed with depleted uranium (tails) makes MOX (Both for French LWRs and ASTRIDs). Reprocessed uranium is unused and stockpiled. Uranium is reprocessed in order to separate the raffinate (minor actinides and fission products) from usable material. Though neglected in this work, reprocessed uranium may substitute depleted uranium for MOX production. In the simulations, sufficient depleted uranium existed that the complication of preparing reprocessed uranium for incorporation into reactor fuel was not included. However, further in the future where the depleted uranium inventory drains, reprocessed uranium (or, natural uranium) will need to be utilized.

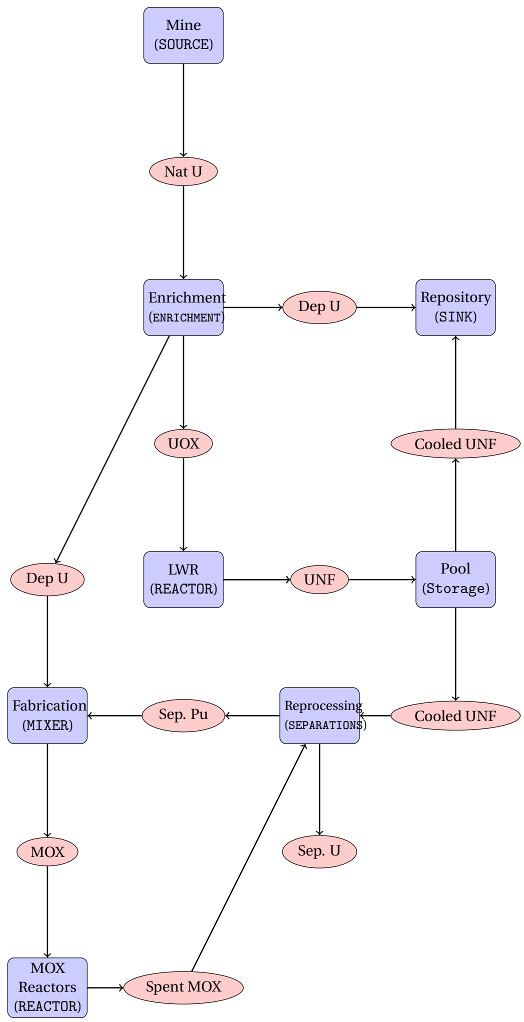

Figure 6.5: Fuel cycle facilities (blue boxes) represented by CYCLUS archetypes (in parentheses) pass materials (red ovals) around the simulation.

6.4 Scenario Specification

The scenario specifications defining the simulations presented in this work are listed in table 6.3. The reprocessing and MOX fabrication capacity in France prior to 2020 is modeled after the French La Hague and MELOX sites [10, 64].

Table 6.3: Simulation Specifications

Specification	**Value**	**Units**
Simulation Starts	1970	year
Simulation Ends	2160	year
Production of ASTRID fuel begins	2020	year
SFRs become available	2040	year
Reprocessed uranium usage	Storage	-
Minimum UNF cooling time	36	months
Separation efficiency of U and Pu	99.8	%
Reprocessing streams	Pu and U	-
Reprocessing capacity before 2020	91.6 [10]	$\frac{\text{metric tons of UNF}}{month}$
Reprocessing capacity after 2020	183.2	$\frac{\text{metric tons of UNF}}{month}$
LWR MOX fabrication throughput	16.25 [64]	$\frac{\text{metric tons of MOX}}{month}$
ASTRID MOX fabrication throughput	No limit (∞)	$\frac{\text{metric tons of MOX}}{month}$
LWR MOX recycling	Not reprocessed	-
ASTRID MOX recycling	∞-pass	-

6.5 Reactor Specifications

Three major reactors are used in the simulation, PWR, BWR, and ASTRID-type SFR reactors. The PWR and BWR specifications are determined using the linear core size model, as explained in section 4.1. The ASTRID-type SFR specification is obtained from Varaine et al [65].

Table 6.4: Baseline LWR and ASTRID simulation specifications.

Specification	**PWR [66]**	**BWR [67]**	**SFR [65]**
Lifetime [2] [y]	60	60	80
Cycle Time [mos.]	18	18	12
Refueling Outage [mos.]	2	2	2
Rated Power [MWe]	1110	1000	600
Assembly mass [kg]	446	180	–
Batch mass [kg]	–	–	5,568
Discharge Burnup [GWd/tHM]	51	51	105
Assemblies per core [3]	157	764	–
Batches per core	3	3	4
Initial Fissile Loading [t]	3.1 ^{235}U	4.2 ^{235}U	4.9 Pu
Fuel	UOX or MOX	UOX	MOX

6.6 Material Definitions

Depletion of the nuclear fuel is modeled with pre-calculated spent fuel recipes, such that a fresh and used fuel recipe are defined for each reactor type. An ORIGEN reference calculation provides the composition of the used fuel.(see table 9.1). ORIGEN calculates buildup, decay, and processing of radioactive materials [68]. This recipe has also been used for repository performance modeling [69].

Table 6.5: Fresh fuel compositions in the simulation [69, 65].

	Composition [%]		
Recipe	U-235	U-238	Pu
Fresh UOX Fuel	3.1	96.9	-
Fresh LWR MOX Fuel	0.2	90.7	9.1
Fresh ASTRID Fuel	0.2	77.7	22

[2] The simulated reactor lifetime reaches the licensed lifetime unless the reactor is shut down prematurely.
[3] Number of assemblies and corresponding LWR core masses are reported for a 1100-MWe core. Reactors with different core powers are modeled with a linear mass assumption.

6.7 Results - Transition Scenario

This section describes the simulation results if France utilized UNF from other EU nations to fuel the transition into a fully ASTRID fleet.

Nuclear Fuel Material Inventory

Table 6.6 lists predicted EU material inventory in 2050. While UNF continues to accumulate after 2050, the UNF France receives before 2050 is most impactful for the feasibility of the transition. Note that table 6.6 distinguishes the stored UNF from the UNF reprocessed to create MOX.

Table 6.6: EU nuclear material inventory in 2050.

Category	**Value [MTHM]**	Specifics
UOX Loaded	161,894	UOX used in EU (minus France) reactors 1970-2050
MOX Loaded	6,945	MOX used in French reactors 1970-2050
Available used UOX (EU)	95,193	Used EU (minus France) UOX in storage for future ASTRID MOX production
Available used UOX (France)	10,029	Used French UOX stored for future ASTRID MOX production.
Reprocessed UOX (France)	53,590	Used French UOX already reprocessed for the production of LWR MOX
Tails	980,294	(Tails generated) − (Tails used for production of LWR MOX)
Natural U Used	1,142,189	

Figures 6.6 and 6.8 show the accumulation of tails and used fuel over time in the EU. Tails accumulate as a by-product of uranium enrichment. For every ton of UOX fuel, about nine times of tails is produced. Spent fuel is discharged from reactors every refueling period. The entire core is discharged when the reactor decommissions. A total of about $1,000,000$ MTHM of tails and $100,000$ MTHM of UNF have accumulated by 2050. Figure 6.7 shows the amount of fuel used in the EU. The tails mass accumulation rate is fairly steady, with peaks occurring when new reactors are deployed. In fig. 6.8, the peaks are caused by reactor decommissioning which triggers all the batches in the final reactor core to be sent to the repository.

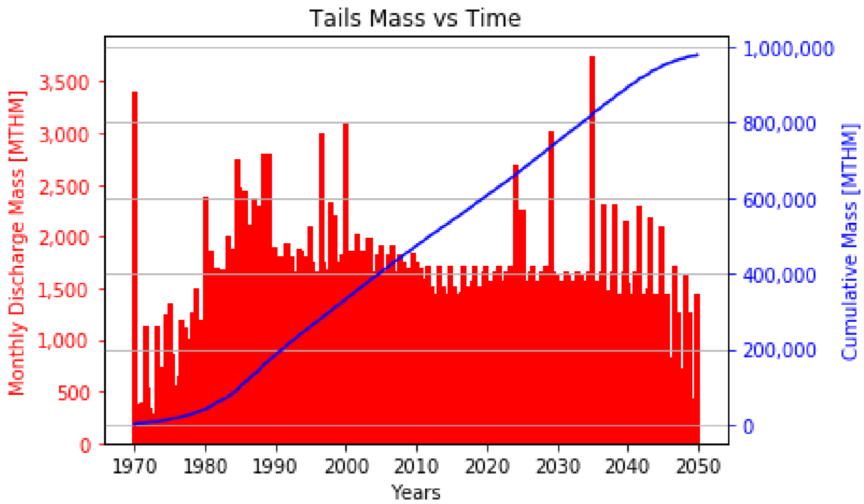

Figure 6.6: Simulated accumulation of tails in the EU is shown as a function of time.

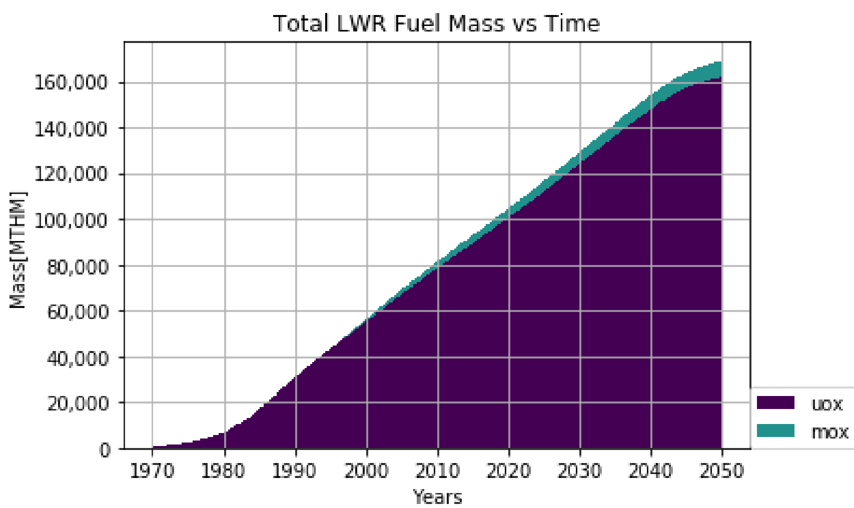

Figure 6.7: Simulated total EU fuel usage is shown as a function of time.

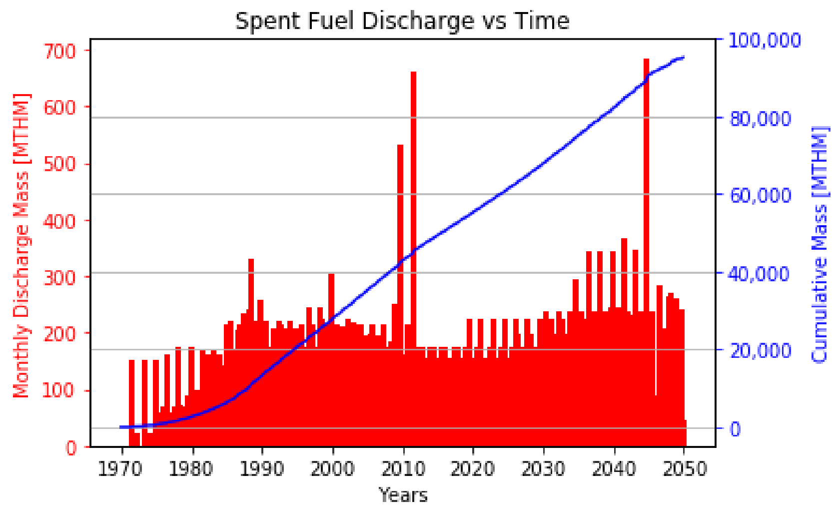

Figure 6.8: Simulated EU UNF accumulation and discharge is shown as a function of time.

French SFR Deployment

Reprocessing the UNF collected from all EU nations can provide the initial cores for approximately 180 SFRs. Table 6.7 lists the isotope, mass fraction, and quantity of plutonium that can be obtained from the 2050 UNF inventory. With the SFR breeding ratio above one, France can transition into a fully SFR fleet without extra construction of LWRs.

Table 6.7: Plutonium in the UNF inventory.

Isotope	**Mass Fraction in Used Fuel [%]**	**Quantity [t]**
Pu238	0.0111	10.52
Pu239	0.518	545.05
Pu240	0.232	244.11
Pu241	0.126	132.58
Pu242	0.0487	51.24
Total	**0.9358**	**983.52**

From Varaine et al. [65], a French ASTRID-type 600MWe SFR consumes 1.225 metric tons of plutonium a year, with an initial plutonium loading of 4.9 metric tons. Thus, the number of SFRs that can be loaded with the reprocessed plutonium from UNF can be estimated to be 200, assuming adequate reprocessing and fabrication capacity as well as abundant depleted uranium supply.

Used MOX from an ASTRID reactor is 23.95% plutonium in this simulation (see table 9.1), whereas fresh MOX is 22% plutonium. The plutonium breeding ratio in this simulation is thus assumed to be ≈ 1.08.

Figure 6.9 shows MTHM of MOX loaded in the SFRs per month. The plot has peaks during a period of aggressive deployment of SFRs followed by an equilibrium at 100 metric ton of heavy metal (MTHM). The peaks reoccur with the deployment of the second generation of SFRs. The spikes are due to initial fuel demand correspoding to these new deployments. The initial cores loaded into new SFRs rely on the MOX created from legacy UNF. Once the deployed SFRs create enough extra plutonium, the legacy UNF is no longer used. Notably, this switch from a less preferred fuel origin to a more preferred fuel origin is handled automatically within CYCLUS via user-defined preferences within its dynamic resource exchange algorithm [70].

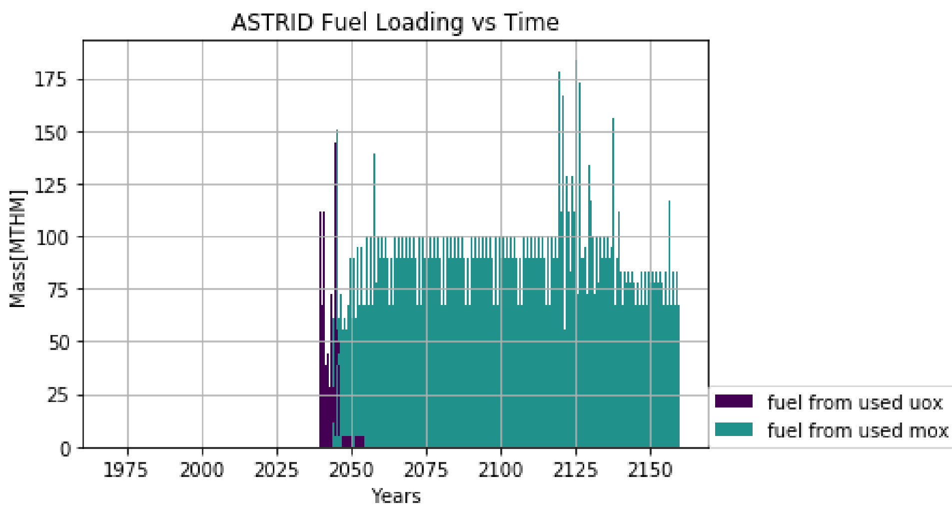

Figure 6.9: Fuel loaded into SFRs was simulated in discrete batches.

Figure 6.10 shows the separated plutonium discharge per month from the reprocessing plant. The plutonium outflux does not precisely follow the fuel demand because CYCLUS agents have material buffers that store commodity fuel for later usage. The reprocessed plutonium from legacy UNF is stored for the initial loading of SFRs. Plutonium separated from legacy UNF meets plutonium demans sufficiently to reduce the reprocessing demand for the first aggressive deployment of SFRs. The plutonium from reprocessing legacy fuel is a flat rectangle because the reprocessing throughput was set to 183.2 $\frac{MTHM}{month}$ to avoid reprocessing all the legacy in one timestep.

Table 6.8 lists metrics obtained from the second simulation.

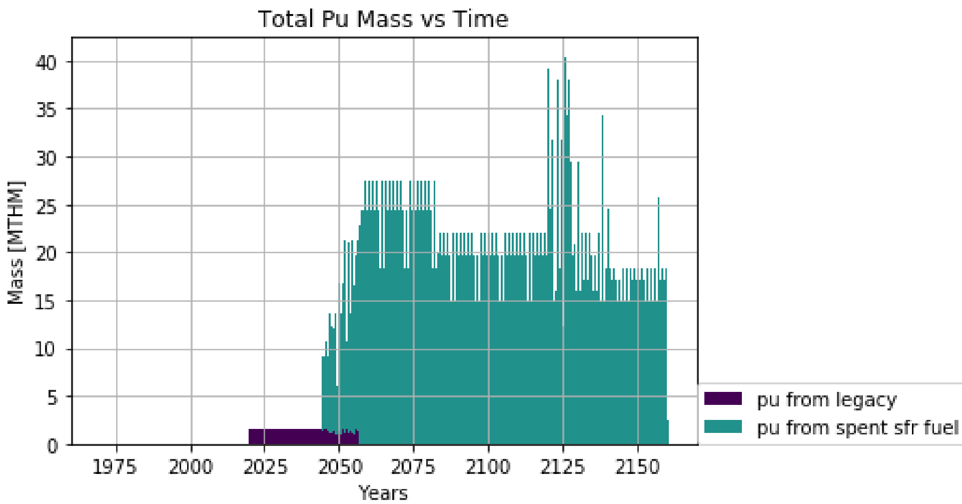

Figure 6.10: The separated plutonium discharge from the reprocessing plant in $\frac{MTHM}{month}$.

Table 6.8: In the French transition to SFRs, the total legacy UNF reprocessed is the amount of UNF France needs for a transition into a fully SFR fleet.

Category	Unit	Value
Total ASTRID MOX used	MTHM	63,447
Average UOX Reprocessing	MTHM/month	**123.27**
Average Total Reprocessing	MTHM/month	**63.23**
Average Fuel Fabrication	MTHM/month	**74.31**
Total SFRs Deployed		220
Total Plutonium Reprocessed	MTHM	14,831
Total ASTRID fuel from UOX Waste	MTHM	2,895
Total ASTRID fuel from MOX Waste	MTHM	60,552
Total Tails used	MTHM	49,488
Total legacy UNF reprocessed	MTHM	**53,595**
Total Reprocessed Uranium Stockpile	MTHM	159,383
Total Raffinate	MTHM	24,789

These results demonstrate that despite the large amount of initial plutonium that has to be reprocessed prior to ASTRID deployment, the 20 years (2020-2040) of ASTRID fuel preparation allows a reasonable level of average UOX reprocessing capacity demand. UOX reprocessing continues until 2057, when the ASTRID spent fuel can supply the plutonium for its own fuel.

6.8 Sensitivity Analysis

I explored the impact of two key variables, the lifetime of French LWRs and the breeding ratio of ASTRID reactors. The range of these parameters (table 6.9) sought to capture the full span of their uncertainty.

Table 6.9: Both LWR lifetime and ASTRID breeding ratio impact transitional reprocessing demand.

Parameter	Default	Values
Breeding Ratio of ASTRIDs	1.08	1.11, 1.15, 1.18
Lifetime of French LWRs [years]	60	65, 70, 80

6.8.1 Breeding Ratio

Increase in the breeding ratio of ASTRID reactors decreases the monthly LWR UNF reprocessing demand, as shown in figure 6.11. An increase in breeding ratio also reduces the number of total UOX UNF required for the transition, because the ASTRID creates more plutonium. The demand previous to 2050 is unaffected by the breeding ratio because only UOX UNF is reprocessed.

The sensitivity analysis also shows, as demonstrated in fig. 6.12 that increasing the breeding ratio decreases the mass of UOX UNF required for the transition. The ASTRIDs produce more plutonium, reducing the plutonium demand from reprocessed UOX.

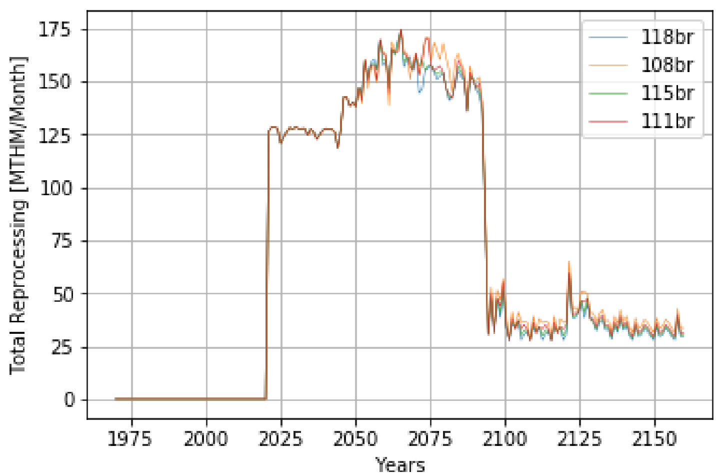

Figure 6.11: Increasing the breeding ratio decreases the monthly reprocessing demand.

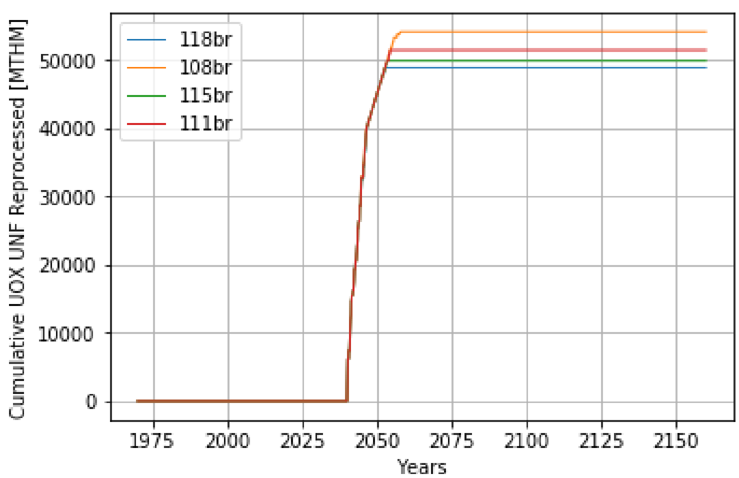

Figure 6.12: Sensitivity analysis demonstrates that increasing the breeding ratio decreases the required UOX UNF.

6.8.2 Lifetime Extension of French LWRs

Extending the lifetime of French LWRs dramatically lowers the average monthly UOX reprocessing demand, since the ASTRID deployment becomes delayed (shown in figure 6.13). The plutonium demand is delayed, allowing the reprocessing plant more time to prepare plutonium for ASTRID reactors.

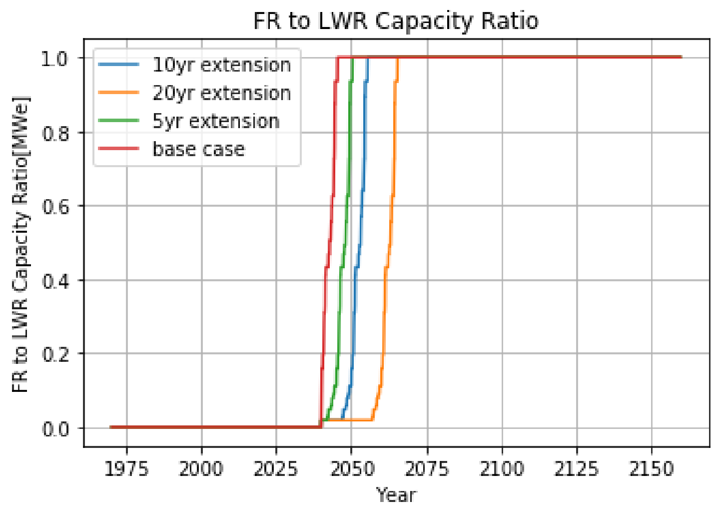

Figure 6.13: The ratio of ASTRIDs to LWRs in France demarcates the transition period.

Increasing LWR lifetimes also enables a less aggressive transition to ASTRIDs. Figure 6.14 shows the decrease in the average monthly UOX reprocessing burden with increased LWR lifetimes, which reduces to the current capacity of the La Hague site if all the French LWRs extended their operation for 20 years. However, figure 6.15 shows that lifetime extension has little effect on the average total monthly reprocessing demand, because the amount of plutonium in the ASTRID used fuel remains the same. The initial increase is caused by the delay of ASTRID deployment delaying the first ASTRID UNF reprocessing. The period of which ASTRID UNF is reprocessed decreases, which increases the average.

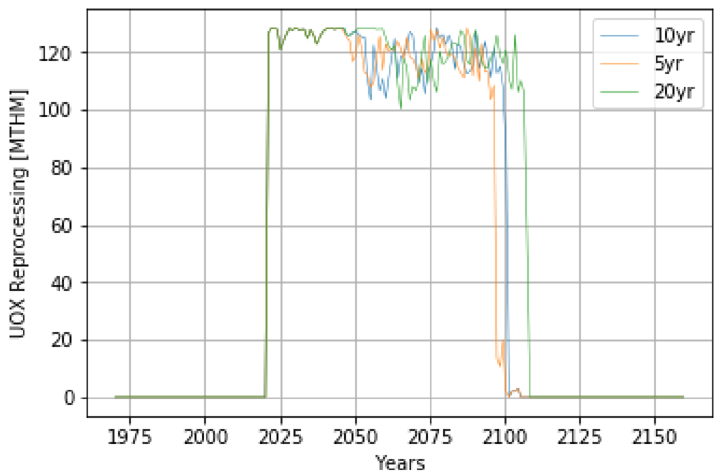

Figure 6.14: Increasing the lifetime of French LWRs decreases the monthly UOX reprocessing demand.

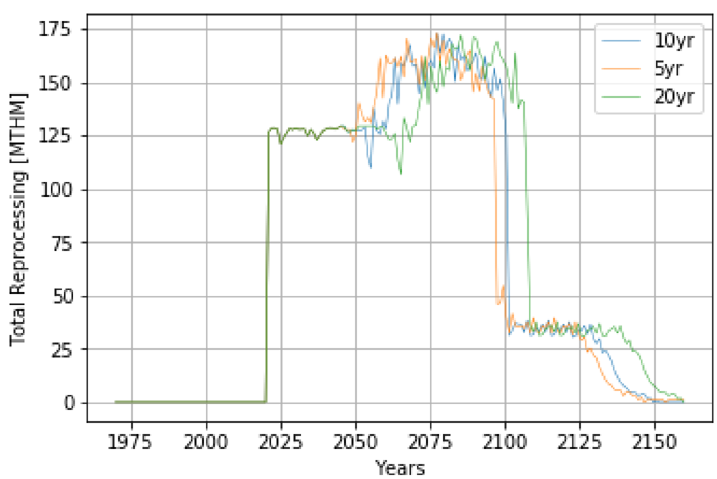

Figure 6.15: Increasing the lifetime of French LWRs simply delays the reprocessing demand, and has little impact on the total reprocessing capacity required.

6.9 Conclusion

France can transition into a fully SFR fleet with installed capacity of 66,000 MWe without building additional LWRs if France receives UNF from other EU nations. Supporting the SFR fleet requires an average reprocessing capacity of 73.27 MTHM per month, and an average fabrication capacity of 45.29 MTHM per month.

Since most EU nations do not have an operating UNF repository or a management plan, they have a strong incentive to send their UNF to France. In particular, the nations planning aggressive nuclear reduction will be able phase out nuclear without constructing a permanent repository. France has an incentive to take this fuel, since recycling used fuel from other nations will allow France to meet their MOX demand without new construction of LWRs.

Table 6.10 lists EU nations and their UNF inventory in 2050. We analyzed a strategy in which the nations reducing their nuclear fleet send their UNF to France. The sum of UNF from Italy, Slovenia, Belgium, Spain and Germany provides enough UNF for the simulated transition ($\approx 54,000$ MTHM). These nations are shown in bold in table 6.10. Sweden is not considered because of its concrete waste management plan.

Table 6.10: EU nations and their respective UNF inventory.

Nation	Growth Trajectory	UNF in 2050 [MTHM]
Poland	Aggressive Growth	1,807
Hungary	Aggressive Growth	3,119
UK	Aggressive Growth	13,268
Slovakia	Modest Growth	2,746
Bulgaria	Modest Growth	3,237
Czech Rep.	Modest Growth	4,413
Finland	Modest Growth	5,713
Netherlands	Modest Reduction	539
Italy	**Modest Reduction**	**583**
Slovenia	**Modest Reduction**	**765**
Lithuania	**Modest Reduction**	**2,644**
Belgium	**Aggressive Reduction**	**6,644**
Spain	**Modest Reduction**	**9,771**
France	**Modest Reduction**	**9,979**
Sweden	Aggressive Reduction	16,035
Germany	**Aggressive Reduction**	**23,868**

On the other hand, in these simulations, some complex political and economic factors were not incorporated and various assumptions were present in this scenario. For example, Germany's current policy is to not reprocess its LWR fuel [71], and this policy would create a shortage in the supply of LWR UNF for ASTRID MOX production. Continuation of that German policy would not, however, be incompatible with a change in EU policy that frees EU countries from creating their high level waste repositories, since France could still agree to take in Germany's UNF for direct disposal. The analysis method described herein could readily be adapted to account for such possibilities. The collaborative option explored here may hold value for the EU nuclear community, and may enable France to advance more rapidly into a closed fuel cycle.

Chapter 7

United States NFC Transition Scenario

The United States has been the forerunner of nuclear energy, with a currently installed nuclear capacity of 99,221 MWe [60]. With its size and long history of nuclear energy, the United States has accumulated about $70,000$ MTHM of UNF.

The complication with modeling the U.S. transition scenario is that the U.S. does not have a defined advanced reactor design, whereas France has a central plan to transition into ASTRID reactors [72, 65]. Previous analyses [35, 34] of the United States NFC transition scenario assumed transition to fast-spectrum SFRs. However, the fact that the U.S. nuclear reactor fleet is decided by economic interests (industries), necessitates exploration of different options, such as transitioning into MSRs.

As explained in section 2.2.3, rising interests in MSR designs led to a proliferation of U.S. corporations aiming to commercialize MSR designs. Given the large interest from industries, MSR designs are most likely to be commercially deployed in the United States.

In this chapter, I explore the U.S. transition scenario from an LWR fleet into an MSR fleet.

7.1 Initial Conditions and Scenario Parameters

For the French scenario, the UNF inventory at the present time is calculated by simulating the nuclear operational history from 1970. However, this is unnecessary for the U.S. scenario because a detailed database exists that describes the U.S. UNF inventory up to May of 2013. The Used Nuclear Fuel Storage Transportation and Disposal Analysis Resource and Data System (UNF-ST&DARDS) is a comprehensive, controlled source of UNF information, including dry cask attributes, assembly data, and economic attributes [73]. This database allows the transition scenario simulation to start from 2013. The UNF inventory mass and composition in 2013 is imported from UNF-ST&DARDS and is 'initiated' in the simulation as a `Source` facility with an inventory of 68,072 MTHM, the total mass of the LWR UNF in the UNF-ST&DARDS.

Furthermore, U.S. currently has additional uranium resources in the form of more than 700,000 MTHM of depleted uranium [74], which is a waste product of enrichment. The depleted uranium inventory is currently a liability and waste, but can be utilized as fertile material in a U-Pu fuel cycle. If the U.S. chooses a Th-^233U fuel cycle, additional thorium resources would be needed, while with a U-Pu cycle, the U.S. can use its waste to create fuel.

The U.S. nuclear fleet in 2013 can be extracted from the PRIS database. The same assumption that legacy reactors have a 60-year lifetime is applied. I used `write_input.py` to generate the expected power capacity of the current U.S. nuclear from 2013 (shown in figure 7.1).

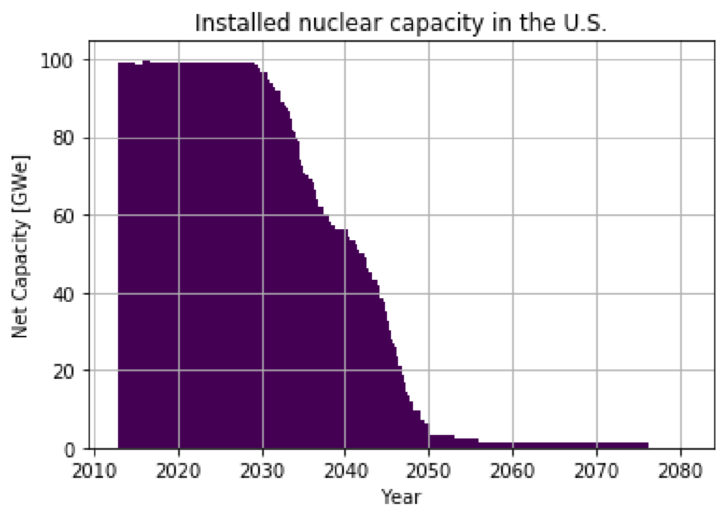

Figure 7.1: Installed nuclear capacity in the United States from 2013.

7.1.1 Energy Demand Prediction

The reference for the energy demand prediction is the U.S. Energy Information Administration (EIA) Annual Energy Outlook [75]. The 2018 Annual Energy Outlook report predicts an annual electricity demand growth of 0.9%. The report also predicts that nuclear power will either remain static or decrease. The report predicts that nuclear capacity will decrease from 99 GWe to 79GWe in 2050, with no new plants beyond 2020. However, for this work, I assume that the U.S. nuclear power capacity is kept at the current capacity of 99GWe, and new reactors are deployed to make up for the decommissioned capacity.

7.1.2 MSR Design and Availability

MSR designs can be categorized depending on their operating neutron spectrum (e.g. fast, thermal), fuel cycle (e.g. Th-^{233}U, U-Pu), and transmutation goals (e.g. breeder, burner). Selection of an MSR design depends on factors like economics, safety, and fuel cycle considerations. For this work, I choose a fast, U-Pu cycle, burner MSR design named REBUS-3700 [44] to deploy for the transition analysis.

The REBUS-3700 MSR design offers five principal advantages over other MSR designs:

- Fast spectrum - no need for moderator rods
- U-Pu cycle - requires only depleted uranium for supply after initial fuel salt loading
- Weakly positive breeding gain (0.03)
  - Self-sufficient (no external fissile input)
  - No surplus fissile material production (stabilizes Pu inventory)
- U-TRU initial fuel - transmutation of long-lived actinides
- Simpler design - no radial / axial blanket

The U.S. has a large inventory of LWR UNF and tails. The benefits of the REBUS-3700 design aligns with the waste management interest of the U.S of reducing final geological repository burden, which can be accomplished by:

- Reduction of TRU inventory by transmutation in the reactor (table 7.1)
  - Reduction of long-term decay heat and activity (figure 1.1)
  - More 'tailored' waste form design for fission products
- Reducing tails inventory

Additionally, the REBUS-3700 does not have, at any moment in operation, separated fissile streams, like other MSR designs such as the Molten Salt Breeder Reactor (MSBR) design [76] (separated ^{233}U), or the Molten Chloride Salt Fast Reactor (MCSFR) design [77] (separated Pu stream from the blanket region). The REBUS-3700 only takes in depleted uranium and processes out fission product groups such as volatile gases and noble metals. The detailed reprocessing scheme is shown in table 7.2. This self-sustained and closed operation increases its non-proliferation properties.

The initial fuel and equilibrium TRU isotopic composition of REBUS-3700 is shown in table 7.1. The TRU isotopic composition matches that of the LWR UNF after 8.5 years of decay (shown in figure 7.2).

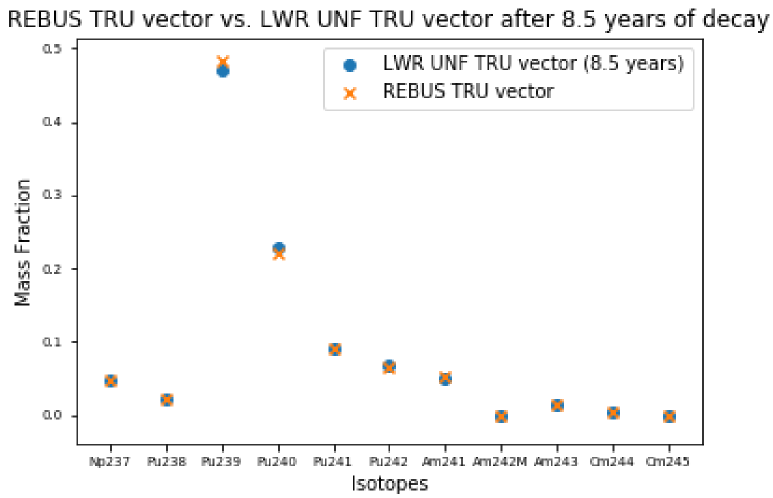

Figure 7.2: TRU vector of REBUS-3700 initial fuel from Mourogov et al. [44] with LWR UNF after 51 GWdth/MTHM burnup and 8.5 years of decay

7.2 U.S. Deployment Schedule

As shown in figure 7.1, the U.S. will undergo a large loss of nuclear capacity from 2030, under the assumption that U.S. reactors have a lifetime of 60 years.

Since it is unlikely that MSRs are ready for commercial deployment in 2020, I deploy LWRs (AP 1000 design [66]) to make up for the decommissioned capacity. After 2050, REBUS-3700 design MSRs are deployed. The deployment of new reactors are shown in figure 7.4, and the installed power capacity of the reactors is shown in 7.3. In the simulation, 84 additional LWRs and 95 MSRs are deployed.

7.3 Material Flow

The fuel cycle is represented by a series of facility agents whose material flow is illustrated in figure 7.5, along with the CYCLUS archetypes that were used to model each facility.

The U.S. transition scenario's material flow is similar to that of France, except that all TRU is reprocessed from LWR UNF to fabricate fuel salt. Also, the depleted uranium from the enrichment plant is stored in a storage facility to be used as a fertile stream for MSR facilities. Natural uranium is mixed with the reprocessed TRU to create fuel salt. Lastly, instead of a single stream of MOX UNF from the MOX reactors, the MSR outputs two streams - waste and end-of-life salt - which are both disposed.

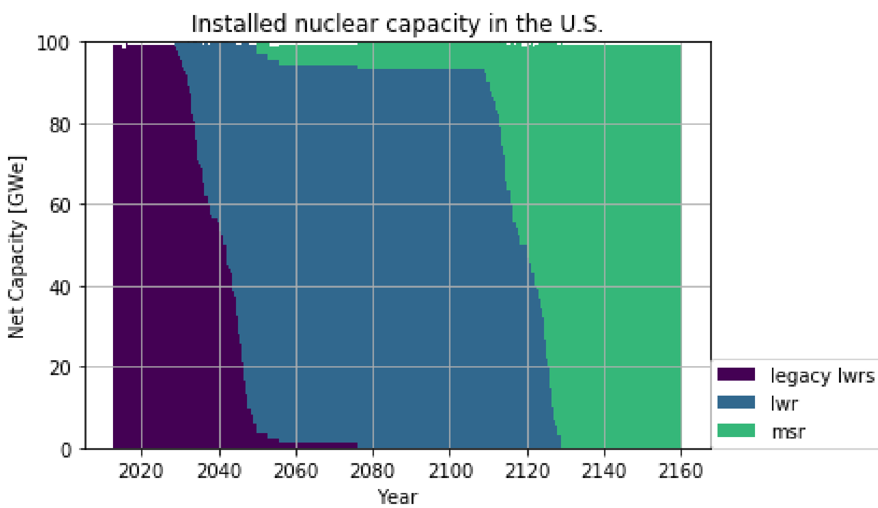

Figure 7.3: Power capacity separated by reactor type from 2020.

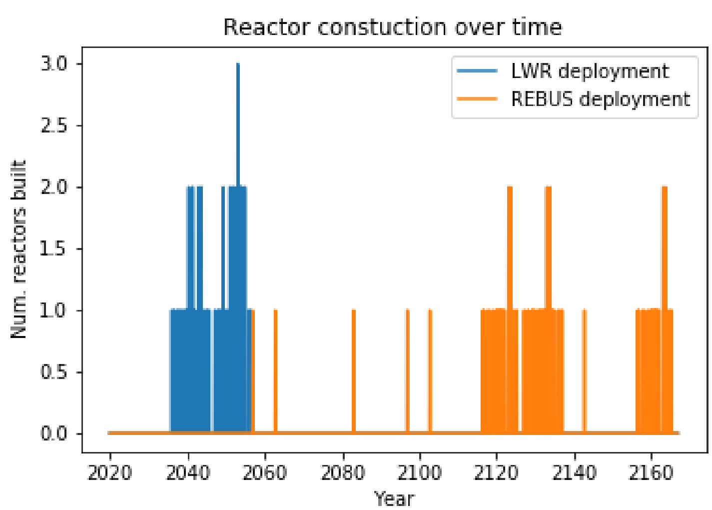

Figure 7.4: New reactor deployment from 2020.

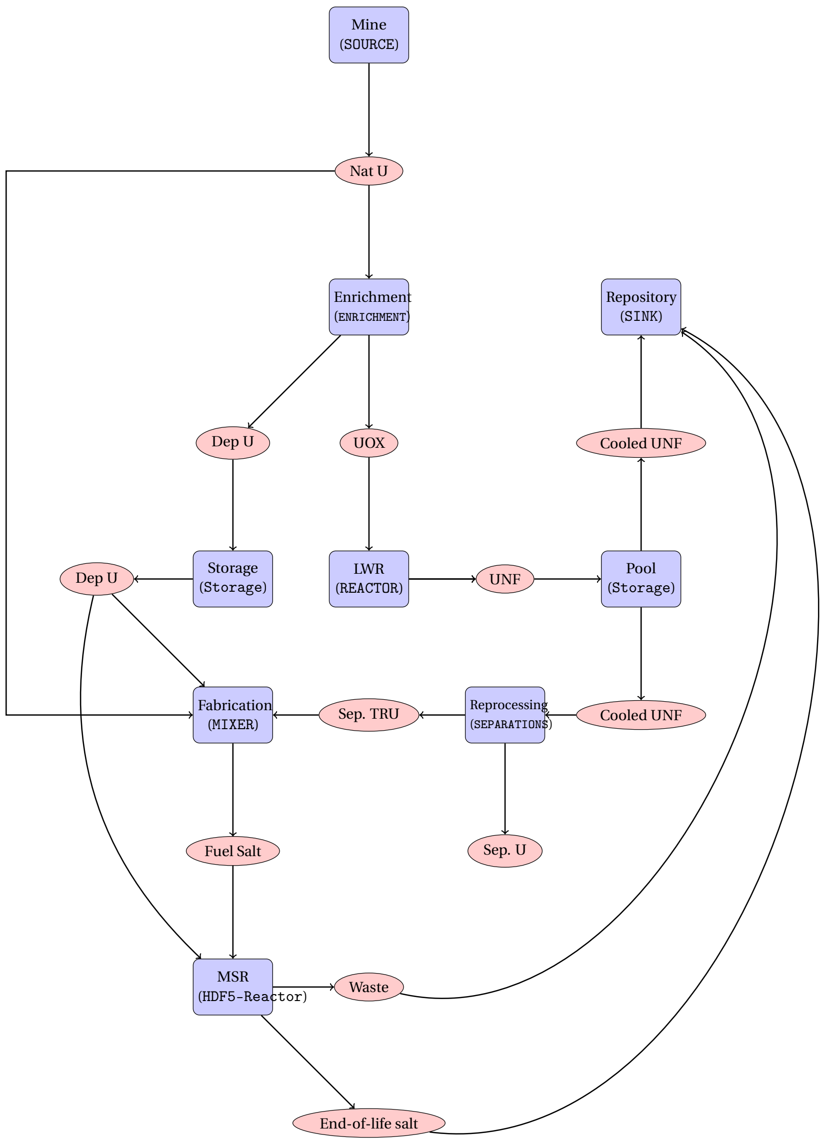

Figure 7.5: Fuel cycle facilities (blue boxes) represented by CYCLUS archetypes (in parentheses) pass materials (red ovals) around the simulation.

Table 7.1: Initial and equilibrium TRU isotopic composition from Mourogov et al. [44].

Isotope	Beginning of Life	Equilibrium (~6500 EFPD)
^{237}Np / ^{239}Np	4.80 / 0.00	0.65 / 0.07
^{238}Pu / ^{239}Pu	2.13 / 48.33	2.23 / 58.02
^{240}Pu / ^{241}Pu / ^{242}Pu	22.17 / 9.05 / 6.38	27.63 / 3.35 / 4.05
^{241}Am / ^{242m}Am / ^{243}Am	5.17 / 0.01 / 1.48	1.50 / 0.12 / 1.05
^{242}Cm / ^{243}Cm	0.0 /0.0	0.07 / 0.01
^{244}Cm / ^{245}Cm / ^{246}Cm	0.43 / 0.04 / 0.00	1.02 / 0.19 / 0.05
Equivalent enrichment, %	10.1	11.0
TRU fraction in heavy atoms, %	15.6	15.9

Table 7.2: Reprocessing scheme for REBUS-3700

Group	Elements	Reprocessing Time (s)
Volatile Gases	Kr, Xe, Ar, Ne, H, N, O, Rn	30
Noble Metals	Se, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Sb, Te, Zr, Cd, In, Sn	30
Rare Earths	Y, La, Ce, Pr, Nd, Pm, Sm, Gd, Eu, Dy, Ho, Er, Tb, Ga, Ge, As, Zn	259,200

7.4 Scenario Specification

The scenario specifications defining the simulations presented in this chapter are listed in table 7.3.

Table 7.3: Simulation Specifications

Specification	**Value**	**Units**
Simulation Starts	2013	year
Simulation Ends	2160	year
Production of MSR fuel begins	2030	year
MSRs become available	2050	year
Reprocessed uranium usage	None	-
Minimum UNF cooling time	8.5	years
Separation efficiency of U and Pu	99.8	%
Reprocessing streams	TRU and U	-
Reprocessing capacity	∞	$\frac{\text{metric tons of UNF}}{month}$
MSR fuel salt fabrication throughput	No limit (∞)	$\frac{\text{metric tons}}{month}$

7.5 Reactor Specifications

Two major reactors are used in the simulation, PWR and MSR.

For PWRs, I use a linear core size model to capture varying reactor capacity (explained in section 4.1). The reactors deployed after 2020 are modeled after the AP-1000 reactor [66]. The reactor specifications are shown in 7.4.

Table 7.4: Baseline LWR and MSR simulation specifications.

Specification	**PWR [66]**	**MSR [44]**
Lifetime [y]	80	40
Cycle Time [mos.]	18	continuous
Refueling Outage [mos.]	2	N/A
Rated Power [MWe]	1110	1628
Assembly mass [kg]	446	N/A
Batch mass [kg]	23,192	N/A
Core mass [kg]	70,022	200,100
Discharge Burnup [GWd/tHM]	51	N/A
Assemblies per core	157	N/A
Batches per core	3	N/A
Initial Fissile Loading [t]	3.1 ^{235}U	19.13 TRU
Fuel	UOX	TRU-U Cl Salt

7.6 Material Definitions

Depletion calculations for the LWR nuclear fuel are recipe-based, such that a fresh and used fuel recipe is calculated beforehand using ORIGEN (see table 9.1). ORIGEN calculates buildup, decay, and processing of radioactive materials [68]. This recipe has also been used for repository performance modeling [69]. For fresh LWR fuel, I assume a fuel enrichment of 3.1% U235.

For depletion calculations for MSR fuel, I use Saltproc (section 3.2) to obtain depleted fuel compositions and waste stream composition in a continuously reprocessing reactor operation. The initial composition for the REBUS-3700 reactor is shown in table 7.5.

7.7 Database Generation

The database used to model MSRs is generated using Saltproc with a unit cell model of the REBUS-3700 reactor. The parameters used for running SERPENT and Saltproc are shown in table 7.6.

The change in K_{eff} values in the REBUS-3700 core in its lifetime is shown in figure 7.6. A lifetime of 40 years is set for the REBUS-3700 reactor since the k_{eff} value drops below 1.01 after 40 years of operation, according to the Saltproc results. The REBUS reactor discharges waste (reprocessed elements - in table 7.2) at an average rate of 90.34$\frac{kg}{month}$ (figure 7.7).

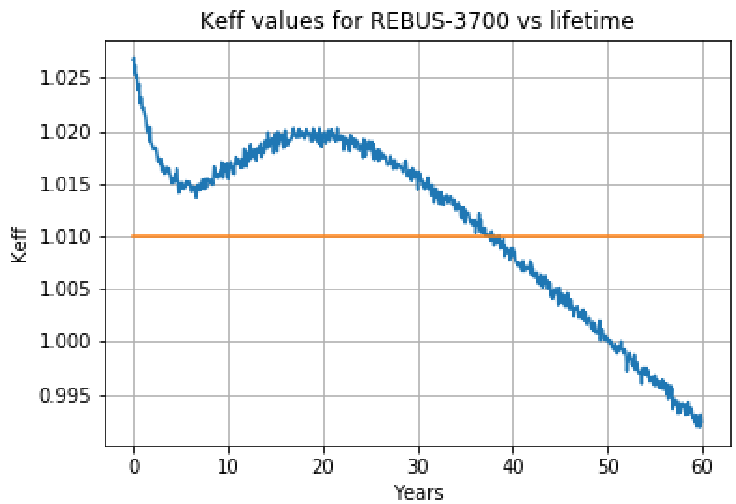

Figure 7.6: Change in K_{eff} value in the REBUS-3700 core. The K_{eff} drops below 1.01 after 40 years of operation.

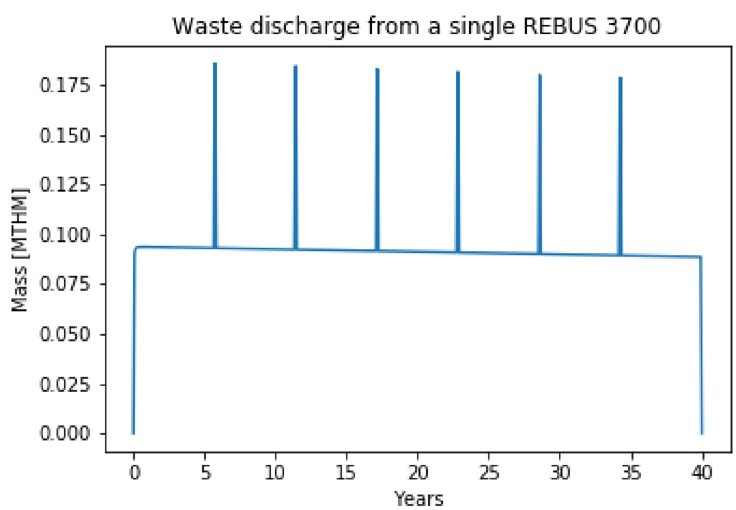

Figure 7.7: Mass of waste discharged from a single REBUS reactor. The peaks are due to the timestep differences in Cyclus and Saltproc, where Cyclus uses 30.43 days for a month (1/12 of 365.25), and Saltproc uses 30-day timesteps. The peaks occur when two Saltproc timestep-worth of waste is discharged per one Cyclus timestep.

Table 7.5: Initial fuel salt composition for REBUS-3700

Isotope	**Mass %**
Na23	6.752
Cl35	26.753
Cl37	9.227
U235	0.343
U238	47.362
Np237	0.459
Pu238	0.204
Pu239	4.623
Pu240	2.12
Pu241	0.866
Pu242	0.61
Am241	0.494
Am243	0.142
Cm244	0.041
Cm245	0.004

Table 7.6: Saltproc simulation parameters used to generate the database for REBUS-3700

Parameter	**Value**
SERPENT Parameters	
Num. neutrons per generation	8,000
Num. active generation	150
Num. inactive generation	50
Burnup calc. mode	CRAM
Power density	$32.18e-3\ \frac{kW}{g}$
Depletion step	30 days
Fuel salt density	$3.6\frac{g}{cm^3}$
Saltproc Parameters	
Lifetime [y]	60
Total timesteps	730
Reprocessing Scheme	As table 7.2
Refill material	Depleted uranium (0.3% ^{235}U)

7.8 Results

Results show that the United States can transition into a fully MSR fleet, while reducing final repository burden by reducing TRU and depleted uranium inventory.

7.8.1 LWR UNF inventory

Table 7.7 lists the U.S. LWR UNF inventory. Since major deployment of MSRs do not begin until 2110, the U.S. has a long time to prepare and accumulate the TRUs required for MSR fuel salt fabrication. The U.S. accumulates an additional 78,281 MTHM of LWR UNF from 2013 to 2130, the year when the last LWR decommissions. Figure 7.8 shows the accumulation of LWR UNF. This figure does not subtract the LWR UNF reprocessed.

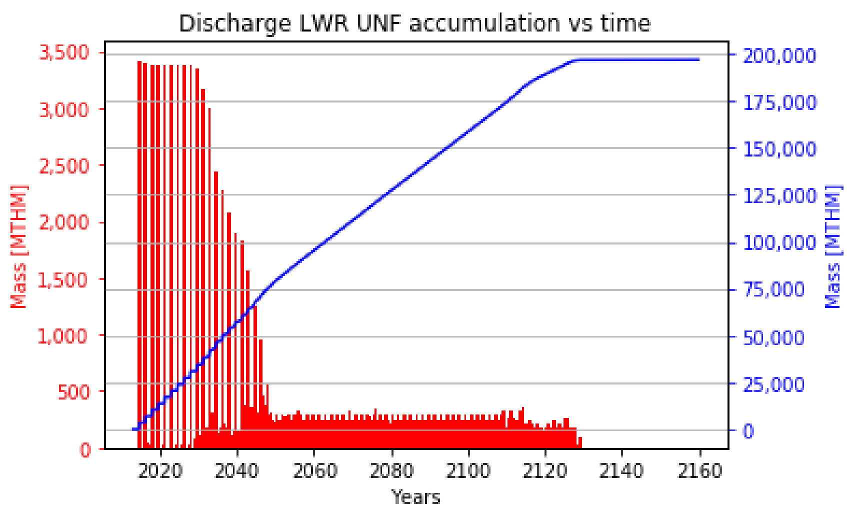

Figure 7.8: U.S. LWR UNF accumulation. The red is the mass discharged per timestep, and the blue is the cumulative inventory. The large discharge quantity prior to 2040 is because the legacy LWRs are deployed in the first timestep, thus discharging their fuel in sync. The later deployed LWRs are not in sync, which makes the monthly discharge values more averaged out.

7.8.2 Reprocessing and fabrication material flow

Metrics for LWR UNF reprocessing is shown in table 7.8. A total of 19,015 MTHM of fuel salt is sent to MSRs. A total of 134,927 MTHM of LWR UNF is reprocessed to extract the TRU for the fuel.

Figure 7.9 shows the cumulative quantity of LWR UNF reprocessed over time. The initial stage (2050-2100) is characterized by a small amount of reprocessing due

Table 7.7: U.S. LWR UNF material flow and inventory

Category	Value [MTHM]
US UNF UOX generated in 2013-2050	78,281
US legacy LWR UNF in 2013	68,072
Total US LWR UNF inventory in 2050	146,353
Total US LWR UNF created from 2013	196,976
Total US LWR UNF created in U.S.	265,048

to the small number of MSRs deployed. On the other hand, from 2100, aggressive deployment of MSRs causes a large increase in the amount of LWR UNF reprocessing. This sudden jump in demand is mediated by reprocessing the LWR UNF beforehand.

Table 7.8: U.S. reprocessing metrics

Category	Value [MTHM]
Total fuel salt mass sent to MSRs	19,015
Total TRU extracted from LWR UNF	1,815
Total LWR UNF reprocessed	134,927
Average monthly reprocessing demand of LWR UNF	94.15
Average monthly fabrication of fuel salt	13.26
Total raffinate stockpile	4,024

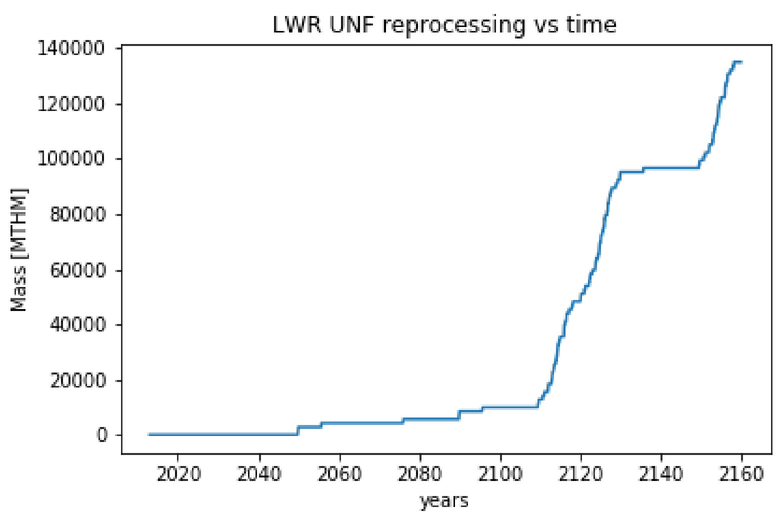

Figure 7.9: The Cumulative mass of LWR UNF reprocessed for MSR salt fabrication.

7.8.3 Waste inventory and resource usage

Table 7.9 shows the mass of various nuclear waste inventory at the end of the simulation. Large quantities of LWR UNF (132,094 MTHM) and depleted uranium (1.1 million tons) remain unused, meaning that more MSRs could have been deployed. The tails usage from the MSRs is not significant compared to the quantity of tails accumulated (0.2% of the total tails inventory). One way to use more tails is to use depleted uranium instead of natural uranium for initial fuel salt fabrication. This would mean increasing the TRU composition in the fuel salt to make up for the decrease in ^{235}U, which is favorable, since there is still 132,094 MTHM of LWR UNF leftover to extract TRU from.

Figure 7.10 shows the monthly discharge and cumulative inventory of waste from MSRs. The discharge mass increases with MSR deployment. The mass of depleted uranium sent to MSRs coincides with the waste outflux, since the mass in the MSR is kept constant.

Table 7.9: U.S. waste metrics.

Category	**Value [MTHM]**
LWR UNF leftover inventory	130,120
Total waste from MSRs	2,972
Total tails created from 2013	1,192,722
Total reprocessed uranium stockpile	260,867
Total tails used	2,972
Total remaining tails inventory	1,189,753
Total natural U used	1,389,698

7.9 Conclusion

The United States can transition into a fully MSR fleet with an installed capacity of 100 GWe by 2130. With the deployment scheme used in the simulation, the U.S. will have sufficient time to prepare the fuel salt necessary for major MSR deployment beginning in 2110. Supporting the MSR fleet requires an average reprocessing capacity of 94.15 MTHM per month, and an average fuel salt fabrication capacity of 13.26 MTHM per month.

The deployment of the REBUS-3700 MSR design allows a reduction in final repository burden, by transmuting the TRU and reducing depleted uranium inventory. However, TRU extraction requires more advanced methods than the currently widely-deployed PUREX method. Resource utilization can be improved if depleted uranium is used instead of natural uranium to fabricated initial fuel, since there is still more than a million tons of depleted uranium available at the end of the simulation. This would require a higher TRU concentration in the fuel, which is also plausible since 132.094 MTHM of LWR UNF are still available for reprocessing.

In reality, however, complications with TRU vectors and changes in MSR performance will occur, due to radioactive decay and differences in LWR UNF cooling time.

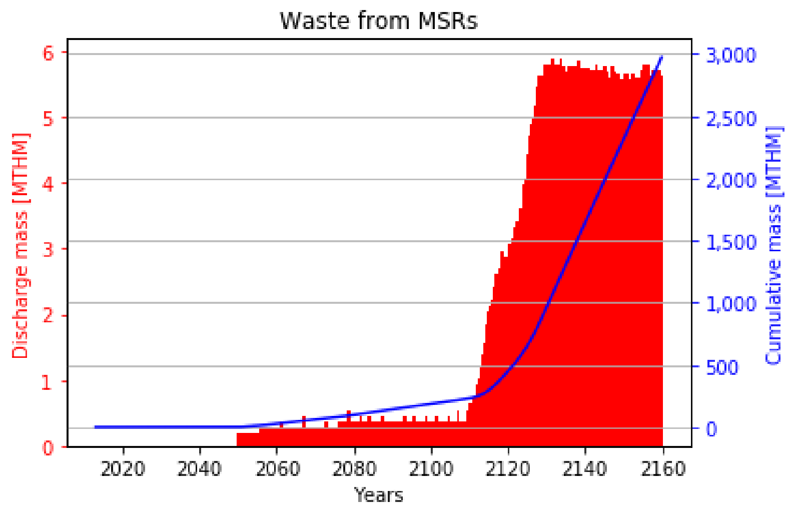

Figure 7.10: Monthly discharged waste and cumulative waste inventory from MSRs. The red bars are monthly discharge values, while the blue line is the cumulative quantity.

This would require careful fabrication of the initial fuel salt so that the desired reactor parameters - multiplication factor, power density - are achieved.

In conclusion, the U.S. can reduce its waste inventory by transitioning into burner MSRs. Choosing a U-Pu cycle instead of a Th-^{233}U cycle eliminates the need to introduce new resources (thorium), usage of moderators, and allows utilization of depleted uranium, which would otherwise be waste. Fissile (separated TRU) and fertile (depleted uranium) material are not limiting factors in the simulation, and a large inventory of LWR UNF and depleted uranium remained at the end of the simulation.

Chapter 8

Conclusion and Future Work

This thesis demonstrates the capability of Cyclus, the agent-based fuel cycle simulator, to model real-world nuclear fuel cycle transition scenarios. Cyclus has a noble framework that is modular and expandable, which allows leveraging its capabilities possible. I developed `write_input.py` to integrate historical nuclear operations by generating a Cyclus input file from a PRIS database. I also developed an MSR module in Cyclus that uses a database generated by a high-fidelity MSR simulation to model an MSR in a large fuel cycle simulation. The two added capabilities leverage Cyclus' existing capabilities to model complex, real-world nuclear fuel cycle transition scenarios.

The Cyclus benchmark study compared Cyclus' results with the results from other fuel cycle simulators (DYMOND [14], VISION [15], ORION [16], and MARKAL [17]) for a generic NFC transition scenario from an LWR fleet to an SFR fleet. Results show excellent agreement, except for disagreement caused by differences in reactor depletion behavior at the end of reactor lifetime, and whether fuel discharge is discrete or continuous.

The France NFC transition simulation demonstrated Cyclus' capacity to model multiple regions' historical nuclear operation. It also showed that France can transition from its LWR fleet into a fully SFR fleet without additional construction of LWRs if France receives LWR UNF from other EU nations.

The U.S. NFC transition simulation demonstrated Cyclus' capacity to roughly model MSRs in a large NFC simulation. The simulation showed that the U.S. can easily transition into a fully MSR fleet, and that availability of nuclear materials (LWR UNF) is not a constraint.

8.1 Future Work

Continued reserach into better methods of modeling fuel cycle transition scenarios and fuel cycle facilities can progress in multiple directions.

First, efforts can be made to incorporate uncertainties in the fuel cycle simulation by adding functionalities in Cyclus where the parameters are governed by an equation or sampled from a distribution. Parameters such as LWR fuel burnup and enrichment evolve in time, and can be better modeled by a function of time than a static parameter. Similarly, reactor parameters such as refuel time and cycle time can be better described by sampling from a distribution (e.g. gaussian) rather than the current static value.

Second, better depletion calculation models can be developed to increase fuel depletion resolution in reactors. The currently used method for LWRs and SFRs are batch-wise, meaning that an average depleted composition is used for the entire batch, while in reality, assemblies in a batch do not have the same burnup.

Third, improvements on the MSR model can be made so that it takes into account the varying initial fuel composition. Due to delays in reprocessing, fuel fabrication, and deployment of MSRs, MSR initial fuels contain varying TRU vectors. This should be taken into account by having a database that contains lifetime depletion calculations of varying initial fuel compositions. Alternatively, an in-simulator depletion module can be developed (if computational resources allow).

8.2 Closing Remarks

The American Nuclear Society (ANS) chose closing the NFC as its grand challenge. ANS proposes to do so by "firmly establish the pathway that leads to closing the nuclear fuel cycle to support the demonstration and deployment of advanced fission reactors, accelerators, and material recycling technologies to obtain maximum value while minimizing environmental impact from using nuclear fuel." The research and development of such technolgoies need to be deliberate. NFC transition scenario simulation and analysis is the first step in identifying technological needs and goals. As demonstrated by this thesis, Cyclus, with its modular structure and expandable nature, is essential in that effort.

Chapter 9

Appendix

9.1 Fresh and Used Fuel Composition

Isotope	Used ASTRID Fuel	Used UOX Fuel	Used MOX Fuel
He4	8.2631E-05	9.4745E-07	2.5108E-05
Ra226	2.306EE-13	9.7885E-14	6.8586E-14
Ra228	6.029EE-21	2.7508E-20	1.0769E-19
Pb206	5.2269E-18	5.5747E-18	3.6378E-18
Pb207	1.0722E-15	1.6859E-15	1.0589E-15
Pb208	4.4347E-10	3.6888E-12	2.0018E-12
Pb210	1.3841E-16	3.0238E-19	1.1829E-19
Th228	7.7910E-10	8.4756E-12	4.9017E-12
Th229	3.5259E-11	2.7278E-12	1.4379E-12
Th230	1.1419E-08	2.6258E-09	2.3998E-09
Th232	6.3415E-11	4.1748E-10	8.7655E-10
Bi209	2.5042E-13	6.6077E-16	2.6878E-16
Ac227	2.8317E-14	3.0968E-14	2.4608E-14
Pa231	8.8076E-10	9.2465E-10	7.0696E-10
U232	1.4693E-07	0.0000	5.9336E-10
U233	4.0461E-08	2.2139E-09	1.0359E-08
U234	0.0010	0.0001	0.0002
U235	0.0003	0.0076	0.0043
U236	0.0005	0.0057	0.0051
U238	0.5864	0.9208	0.8283
Np237	0.0038	0.0006	0.0043
Pu238	0.0096	0.0002	0.0060
Pu239	0.0981	0.0060	0.0410
Pu240	0.0890	0.0029	0.0283
Pu241	0.0155	0.0017	0.0146
Pu242	0.0273	0.0008	0.0098
Pu244	1.779EE-07	2.8648E-08	2.1888E-07
Am241	0.0077	6.4427E-05	0.0021
Am242m	0.0005	8.5336E-07	5.0357E-05
Am243	0.0091	0.0001	0.0020
Cm242	0.0004	2.5898E-05	0.0002
Cm243	0.0000	0.0000	1.2639E-05
Cm244	0.0067	8.5616E-05	0.0010
Cm245	0.0017	5.7217E-06	0.0001
Cm246	0.0009	7.2956E-07	6.1406E-06
Cm247	0.0000	0.0000	1.2059E-07
Cm248	4.0265E-06	7.6916E-10	9.1585E-09
Cm250	1.076EE-12	4.2808E-18	3.7338E-17
Cf249	1.6590E-07	1.6499E-12	4.0567E-11
Cf250	9.5219E-09	2.0419E-12	2.9328E-11
Cf251	3.2032E-10	9.8655E-13	1.4479E-11
Cf 252	8.3754E-12	6.5797E-13	7.5346E-12
H3	3.1829E-07	8.5846E-08	1.0269E-07
Kr81	1.5156E-11	4.2168E-11	7.3446E-11
Kr85	0.0000	3.4448E-05	2.0548E-05
Sr90	0.0009	0.0007	0.0004
Tc99	0.0029	0.0011	0.0011
I129	0.0009	0.0002	0.0003
Cs134	0.0001	0.0002	0.0002
Cs135	0.0051	0.0006	0.0009

Table 9.1: Spent Fuel Compositions

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