State-Level Nuclear Fuel Cycle Simulations for International Safeguards Applications

by

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ABR Advanced Burner Reactor 151, 159, 165

ADS accelerator-driven system 119, 134, 237

ANL Argonne National Laboratory 8, 148, 151, 159, 165

AP Additional Protocol 14, 32, 42, 233–235

APA acquisition path analysis vi, xxix, xxxi, xxxii, 2, 19, 20, 25, 26, 29, 30, 32, 42, 43, 45, 46, 203

API application programming interface 102, 228

B&B breed-and-burn 148, 149, 175

BWR Boiling Water Reactor 133, 161, 174, 175, 184, 197, 239

CANDU CANada Deuterium Uranium 123, 141, 142, 185, 186

CART classification and regression tree 16

CEA Commissariat à l'Énergie Atomique et aux Énergies Alternatives 8

CIS consolidated interim storage 77, 135, 137, 141, 143, 146, 150, 153, 154, 156, 158, 160, 161, 163–165, 167, 168, 170, 192

CNRS Centre national de la recherche scientifique 8

CSA comprehensive safeguards agreement 2, 5, 12–14, 32, 89, 92, 93, 106, 175, 233–235

DA destructive analysis 16

DF discharged fuel 237

DGR deep geologic repository 157

DOE U.S. Department of Energy xxxviii, 10, 122, 133, 135, 139, 187, 189, 233

DRE dynamic resource exchange 26, 47–49, 51, 54, 55, 66, 73, 75, 82–84, 204, 206, 228, 229

DU depleted uranium 38, 97, 99, 115, 116, 150, 152, 153, 174, 175, 188, 189

DUPIC direct use of spent PWR fuel in CANDU 126

E&S *Nuclear Fuel Cycle Evaluation and Screening – Final Report* xxxviii, xxxix, 5, 6, 10, 11, 109–111, 113–115, 118–120, 124, 125, 137, 139, 151, 157, 173

EDS externally-driven system 112, 117, 119, 133, 154–156, 174, 175, 184

EFPD effective full-power days 120, 122, 142, 149

EG evaluation groups 109–113, 118, 139, 141, 143–147, 149–152, 154–157, 159–162, 165, 166, 169, 170, 172–174

EPRI Electric Power Research Institute 162

EU European Union 233

FA Facility Attachment 13, 89–93, 176

FCDP Fuel Cycle Data Package 153, 236–239

FOSS free and open-source software 8

FP fission products 116, 125, 127, 152, 154, 156–158, 160, 164, 165, 167, 170–172, 202

GAIN Gateway for Accelerated Innovation in Nuclear 122

GAO U.S. Government Accountability Office 122

GCEP gas-centrifuge enrichment plant 40

HALEU high-assay low enriched uranium 113, 115, 116, 139, 140, 144–148, 150, 151, 157–160, 165–167, 174, 188

HEU highly enriched uranium 28, 34, 38–40, 115, 116

HLW high level waste 126, 156

HM heavy metal 115, 141, 143, 145, 147, 150, 152, 155, 158, 160, 162, 166, 169, 172

HTGR High Temperature Gas-Cooled Reactor 133, 144, 174, 186

HWR heavy water reactor 5, 108, 111, 133, 141, 174, 175, 185, 189, 194, 196, 197

IAEA International Atomic Energy Agency xviii, xx–xxii, xxiv, xxvi, xxix, xxxi–xxxiv, xxxvi, xxxvii, 1–3, 5, 6, 9, 12–20, 25, 32, 42, 46, 47, 49, 88–92, 101, 103–106, 115, 122, 175, 176, 184–186, 188–191, 201, 202, 205, 233, 235

ICR inventory change report 3, 14, 90–96, 98, 102, 103, 176, 194, 195, 198, 201, 205, 207, 210

IMCI inventory-monitor containment-inventory 186, 187

INFCIRC information circular 12–14, 201, 234

INL Idaho National Laboratory 146

IRSN Institut de radioprotection et de sûreté nucléaire 8

ISL *in-situ* leaching 130, 136

JAERI Japan Atomic Energy Research Institute 190

JCPOA Joint Comprehensive Plan of Action 21

JIT just-in-time 178

KMP key measurement point xviii, 4, 13–15, 49, 91, 92, 100, 103, 176, 185, 192, 193, 196, 200, 204, 208, 209

LANL Los Alamos National Laboratory xxiv, xxxiii, xxxviii, 8, 19, 146

LEU low enriched uranium 28, 40, 111, 115, 116, 139–141, 155, 169, 174, 175, 184, 188, 194, 197

LFR Lead-Cooled Fast Reactor 134

LOF locations outside facilities 13, 14, 32, 42, 89, 233

LWR light water reactor 2, 5, 11, 108, 111, 122, 133, 134, 138, 139, 148, 151, 154, 162, 163, 194

MA minor actinide 118, 125, 153, 156, 159, 160, 162, 164–167, 172, 202, 239

MBA material balance area xviii, xxxvii, 4, 5, 13–15, 25, 30, 33, 48–50, 77, 88, 90–93, 95, 101–104, 165, 170, 175, 176, 184, 185, 187–197, 199–201, 204, 206, 208, 209, 228, 233, 238, 245, 248

MBR material balance report 15, 90, 91, 98, 209

MC&A material control and accounting/accountability 186, 233

MDC material description code 93, 101–105, 195, 196, 200

MIT Massachusetts Institute of Technology 8

MOX mixed oxide 38, 39, 165

MPC multi-purpose canister 138, 185, 238

MSBR Molten Salt Breeder Reactor 170

MSR Molten Salt Reactor 3, 112, 116, 132, 133, 163, 170, 174, 175, 186, 187, 189, 197, 238

MUF material unaccounted for 22, 23, 88, 91, 209

NDA nondestructive assay 16

NFC nuclear fuel cycle 23, 24, 45, 47, 48, 109–111, 113, 120, 192, 236

NFCSS Nuclear Fuel Cycle Simulation System 9

NMAC nuclear material accountancy and control 233

NNL National Nuclear Laboratory 8

NNWS non-nuclear-weapon States xxii, xxvii, xxviii, xxxiii, xxxvi, 12

NNWS non-nuclear-weapon State 12, 14, 175, 190, 204

NPT Treaty on the Non-Proliferation of Nuclear Weapons xx, xxi, xxiv, xxvii, xxviii, xxxii, 1, 12, 14, 17, 18, 24, 88, 204, 234, 235

NRC Nuclear Regulatory Commission 186, 233

NU natural uranium 30, 40, 97, 99, 111, 116, 141–143, 149, 150, 159–166, 169, 170, 174, 175, 188, 194, 197

NWS nuclear-weapon States 235

NWS nuclear-weapon State xxii, xxiv, xxvii, xxviii, 12, 14

ORNL Oak Ridge National Laboratory 8, 170, 186

PIL physical inventory listing 15, 90, 91, 98, 192, 208, 209

PIT physical inventory taking 15

PNC Power Reactor and Nuclear Fuel Development Corporation 190

PNNL Pacific Northwest National Lab 8, 101, 191

PRNG pseudo-random number generator 51, 52, 57, 58, 87

PWR Pressurized Water Reactor 112, 133, 138, 139, 153, 154, 156, 157, 164, 165, 168, 170, 174, 175, 184, 195, 237, 238

QCVS Quality Control Verification Software 105, 248

R&D Research and Development xviii, 13, 16, 32, 92, 125, 130–132, 137, 138, 141, 145, 146, 160, 161, 170

RBWR Resource-renewable Boiling Water Reactor 161–163, 238

RFB Request for Bids 74, 229

RM recycled/recovered material 112, 125, 126, 137, 150, 152, 160, 162, 169, 170, 172, 174

RRFB Response to Request for Bids 74, 82, 83, 86, 228, 229

RSAC regional system of accounting for and control of nuclear material 233

RU reprocessed uranium 115, 116, 125, 126, 150, 152–154, 156–162, 164–167, 169, 174, 194, 239

SBD safeguards by design 3

SFR Sodium-Cooled Fast Reactor 133, 134, 148, 150, 151, 153, 159, 160, 163, 164, 174, 175, 184, 237, 238

SIP Safeguards Implementation Practices 14

SLA State-Level Approach 18

SLC State-Level Concept 17, 18, 26, 27, 38, 88

SME subject matter expert 105

SMR small modular reactor 2, 144, 237

SNL Sandia National Laboratory 186

SNM special nuclear material 130, 132

SPR Special Purpose Reactor 146, 237

SQ significant quantity 20

SQP small quantities protocol 14

SSAC State system of accounting for and control of nuclear material 13, 32, 89, 175, 184, 185, 208, 233

SSFR Sustainable Sodium-Cooled Fast Reactor 148

SSPM Separations and Safeguards Performance Model 23

SWU separative work unit 21, 33, 136

TRISO Tristructural Isotropic 144, 185, 186

TRU transuranics 11, 109, 112, 117, 118, 125, 126, 150–154, 157, 158, 161–163, 165–167, 170, 174, 175, 190, 191, 194, 238, 239

UNF used nuclear fuel 7, 31, 34, 50, 92, 102, 115, 118, 124, 125, 127, 128, 135, 137, 138, 140, 142, 147, 149, 151, 153, 154, 156, 157, 159, 163, 164, 166, 167, 170, 185, 186, 193, 206, 238, 239, 245

UOC uranium ore concentrate 58, 120, 135, 138, 140–143, 145–148, 156, 158

UOX uranium oxide 237

VOA voluntary offer agreements 14, 235

WNA World Nuclear Association 122

XOR exclusive-or 40

ABSTRACT

With more countries considering nuclear power as part of their energy future than ever before, it is critical to ensure that all uses of nuclear materials for commercial nuclear energy are and remain peaceful. With this expanding mission, the International Atomic Energy Agency (IAEA) also faces an increase in data to process, without a correspondingly large increase in analyst time.

Several tools were built on or within the Cyclus nuclear fuel cycle simulation platform that enable system-scale modeling and analysis to aid nuclear safeguards approaches and evaluation. Specifically, this work addresses the lack of real or realistic data on State accountancy reports available to the R&D community by expanding the realistic behaviors able to be modeled within Cyclus (Chapter 4), allowing the tool to track nuclear material using material balance areas and/or key measurement points. Building on the enhanced simulation capabilities added to Cyclus, a tool was developed to generate accountancy reports in the exact style and form of reports submitted to the IAEA, often called Code 10 (Chapter 5). With the wealth of additional tools and capability resulting from these efforts, I demonstrate a new capability to simulate realistic nuclear fuel cycles on a number of systematically created synthetic States (Chapter 6) to aid in the larger mission of developing enhanced techniques for nuclear material accountancy report and declaration processing and diversion detection.

Preface

Science is only useful when it is communicated. Scientific journals and conferences propagate advancements within a discipline and allow scientists to build on each other's work. Events with schools help grow the next generation of scientists, and I can trace my own journey back to science summer programs and opportunities to meet scientists as a kid. General audience media is for everyone to enjoy and explore the new knowledge and capabilities generated each day by scientists and engineers.

For many scientists, however, only the first type of communication counts as part of their jobs unless they can convince high-profile organizations like *Scientific American* to cover their research. But scientific knowledge should be for everyone.

Nuclear engineering has a long and complex relationship with public communication. When the fields of risk communication and decision science were first being developed, nuclear energy, nuclear waste, and nuclear weapons were consistently studied as examples of industrial hazards.

After the Three Mile Island accident in 1979, the nuclear power industry learned to communicate its operational experience across companies (a very good practice that continues today) and to limit its communication to the public to avoid potential communication mishaps (a bad practice that is still being unlearned). The limited public communication strategy backfired, allowing entertaining but not factual portraits of nuclear power like *The Simpsons* and anti-nuclear energy activists to dominate the information ecosystem. The lack of public presence has contributed to the spread of misperceptions and a general lack of awareness of nuclear energy compared to other energy sources. Nuclear engineering has always needed messengers. Here is my story as a nuclear engineer and the story of my dissertation.

This chapter is also part of the Wisconsin Initiative for Science Literacy (WISL) Communicating PhD Research to the Public project. I am grateful to the WISL team, Bassam Shakhashiri, Elizabeth Reynolds, and Cayce Osborne, for creating this project and encouraging Ph.D. students to make sure their work is accessible to a broad audience. They also guided me through this process and edited this chapter, which I greatly appreciate. You can also read dozens of other dissertation general audience chapters on their website.

tl;dr

Over 180 countries have signed the Treaty on the Non-Proliferation of Nuclear Weapons [3], promising never to develop nuclear weapons. We don't just take them at their word, though. In signing the treaty, each country agreed to declare their nuclear materials and facilities and open them up for inspection to an independent agency within the United Nations system, called the International Atomic Energy Agency (IAEA). My dissertation enhances the capabilities of a computer code called Cyclus, which models the movements of nuclear materials throughout their entire lifecycle, to support this verification system.

I demonstrated the ability of Cyclus to "play nicely" in the international safeguards verification system by incorporating an analysis technique that's already used in the field into the Cyclus ecosystem. I dug into the way that nuclear facilities in Cyclus trade nuclear materials between them, adding new capabilities that replicate more complex behavior and overcome prior limitations. I created a tool to convert those simulations into synthetic nuclear material accounting reports using the exact format that countries have to use when they submit their reports to the IAEA. Finally, I created a small set of fake countries that can be used for demonstrations of realistic nuclear material movements without being limited by what exists today.

Together, these capabilities can be used to create synthetic versions of nuclear material accounting reports, which real countries use to record detailed information about their nuclear materials. These synthetic reports can be used to find more efficient ways to implement the IAEA's inspection system, especially useful now with the agency having a strained budget and increasing number of nuclear facilities to inspect. They can also be used to look for previously unknown signatures of nuclear material diverted away from peaceful uses towards a potential nuclear weapons program.

Introduction

I'm part of a global hide-and-seek game, where the stakes could not be higher. Any time a new country develops nuclear weapons, the potential for accidental or intentional use increases.

Let's call any country that wants nuclear weapons the hider. I don't know if or how many hiders even exist. If any do, they have access to an entire nation's resources to stay undetected. I use the analogy of a kid's game, but in the real world, this is deadly serious. Any hiders do *not* want to be found.

Who are the seekers? Well, anyone who doesn't want additional nations with nuclear weapons to exist as a start. But more specifically, the International Atomic Energy Agency (IAEA). This organization is affiliated with the United Nations and tasked with enforcing the provisions of the Treaty on the Non-Proliferation of

Nuclear Weapons (NPT) [3]. Nearly every country in the world is a member of the treaty, which places each signatory nation into one of two categories: nuclear-weapon States, and non-nuclear-weapon States. The IAEA calls countries/nations States with a capital S, which is the terminology used through the rest of the dissertation, but I'll stick with countries here.

In this analogy, I'm not a seeker, I'm more like the seeker's support team. My goal is to find new ways to seek out clandestine nuclear activities. I'm building software that enables researchers to play virtual hide-and-seek, where they get to act as both sides of this adversarial game. By simulating many hypothetical hide-and-seek games, we can hopefully make it easier to detect potential real-life secret nuclear weapons programs.

So how does one end up getting a nuclear engineering Ph.D. in nuclear nonproliferation?

I mentioned that my work is designed to help detect the spread of nuclear weapons technology. We'll return to the story later, there's a lot more to tell. But right now, I want to share with you how I ended up here.

As a kid, I fell in love with the mountains. My dad's family is from central Pennsylvania, in the heart of the Appalachian Mountains. We would visit them every year. Those mountains are old, older than anything humans can really wrap our minds around. They're a product of immense geologic forces. Every mountain stands in defiance of the gravity, wind, and water that seek to pull them back down. I was, and am, awestruck.

These dominating and yet delicate landscapes drew me to a passion for the environment as I grew older. I wanted to study natural systems, I thought. I wanted to be a meteorologist or an astrophysicist. Maybe a geologist studying water systems? I learned that mountains, like every other ecosystem on our planet, are affected by climate change, which spurred my passion even more.

Then, I learned about engineering and decided that I could channel my energy into climate solutions. I could use the power of applied science to protect the natural systems I loved. My attention eventually fell on energy, which powers our modern life. The widespread adoption of electricity, much of it generated from burning coal and other fossil fuels, has enabled many of our technological advances in the past century. Of course, it has also pumped enormous amounts of carbon and other greenhouse gases into the atmosphere.

I believe that we need to build a future that doesn't emit carbon but also allows the entire world to reach the living standards we enjoy in the United States. We need a world powered by clean energy. I sought information about solar, wind, hydro, geothermal, and nuclear energy.

I now know that all kinds of engineers work on climate solutions. But as a 17-year-old, it made sense to pursue a major that was such an obvious pathway to work on clean energy: nuclear engineering. I was lucky to find mentors and role models who helped me see nuclear energy and engineering as a viable degree and career for myself.

It turned out to be a perfect fit for me. Nuclear engineering is very physics-heavy for an engineering field, letting me satisfy my childhood dream of studying complex scientific systems. The field holds so much promise, but there are also many challenges to overcome. I didn't want a slam dunk.

As an undergraduate student, I discovered that I had a passion for interdisciplinary challenges. I loved the pure science and the engineering of my classes, but I was drawn to the socio-political aspects of nuclear energy and engineering in the real world.

It wasn't until the summer after I got my bachelor's degree that I even really thought about nuclear weapons. Nuclear engineering programs train students specifically for careers in nuclear energy or in medicine. Nuclear technology has so many incredible peaceful uses. Although it's common for people to assume that nuclear power plants can blow up like an nuclear bomb, the technologies are designed very differently; even the worst possible nuclear accidents could not cause an explosion like a nuclear weapon. Undergraduate nuclear engineering students are not typically taught about nuclear weapons proliferation or the prevention of nuclear weapons proliferation through nonproliferation.

Nuclear nonproliferation only became a focus of mine when I came to Los Alamos, New Mexico for the first time as an intern at Los Alamos National Laboratory (LANL). I studied the use of nuclear thermal rockets for space power, but I also learned nuclear history. Known as the birthplace of the atomic bomb, Los Alamos played a pivotal role in the Manhattan Project (have you seen Oppenheimer?).

"[N]uclear war cannot be won and must never be fought". U.S. president Ronald Reagan and then-Soviet president Mikhail Gorbachev made this statement in 1985, and it's still powerful, and true, today. It is so important that the five nuclear-weapon State signatories of the NPT, the U.S., France, U.K., Russia, and China have recently released a joint statement re-affirming the phrase.

That summer, I learned about the Treaty on the Non-Proliferation of Nuclear Weapons. I learned that the IAEA is still checking to make sure that countries that signed the treaty as non-nuclear weapons States are holding up their end of the bargain. And I found a way to think about climate change and nuclear weapons together as two existential threats to humanity.

I joined the hide-and-seek game.

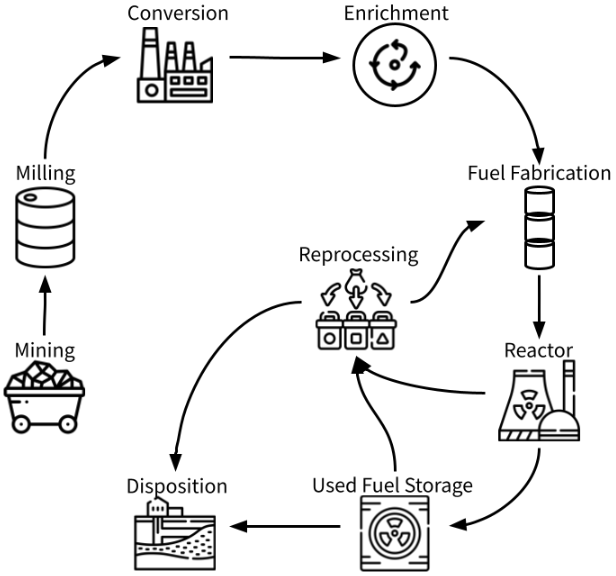


Figure 0.1: The nuclear fuel cycle starts with mining of uranium and/or thorium and ends with disposal of nuclear materials. Reprocessing can be used to recycle used nuclear fuel for additional use in a reactor, which is called a closed nuclear fuel cycle. Otherwise, the fuel cycle is called open.

The uranium lifecycle

My work brings together two different applications of nuclear engineering that have historical overlap but have long since diverged. I'll introduce them separately and then tell you how I brought them together and what my work enables.

Although I bridge two disciplines, I consider myself first and foremost an expert in nuclear fuel cycle modeling. The nuclear fuel cycle is a technical term for the lifecycle of nuclear materials like uranium. This encompasses all the steps from digging up uranium-bearing ore from the ground to the chemical processing that turns rock into highly refined nuclear fuel assemblies, to the reactor itself, where uranium is split in two by a process called nuclear fission, to the final permanent disposal of nuclear fuel back underground.

Much of nuclear engineering is focused on the nuclear chain reaction occurring in the reactor core and all the complicated processes that are needed to build and maintain a nuclear reactor and turn the energy from nuclear fission into usable electricity. My work in the nuclear fuel cycle is instead focused on the supply chain of nuclear materials that fuel the reactor and is responsible for the used nuclear fuel afterwards.

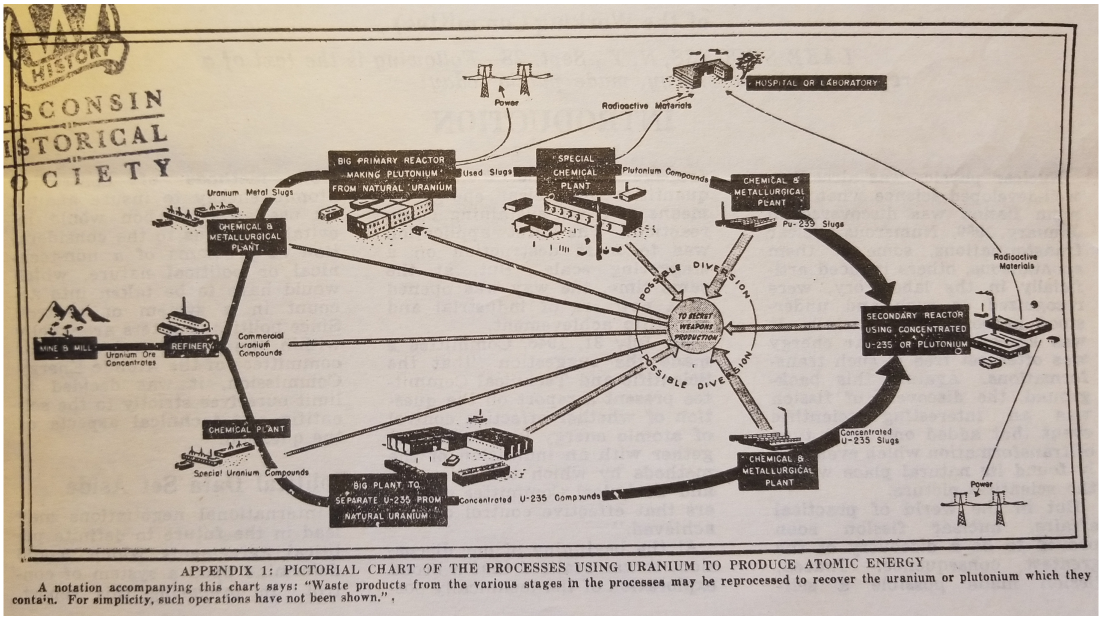
I went to graduate school specifically to pursue nuclear fuel cycle modeling. From my earliest days as an undergraduate in nuclear engineering, I was drawn to the complex system that supports energy-producing nuclear reactors.

International nuclear safeguards, the global hide and seek game

At the advent of the nuclear age, in 1945, only one country had nuclear weapons. The United States developed nuclear weapons in the secret Manhattan Project during WWII. The U.S. announced their existence by deciding to drop two nuclear bombs on Japan, killing between 110,000 and 210,000 people depending on the source and their assumptions [4].

U.S. President Dwight D. Eisenhower gave his famous "Atoms for Peace" speech in 1953, leading to the creation of the IAEA as an independent agency within the United Nations family. The IAEA was created to promote peaceful uses of nuclear technology, which are now entrenched in modern life. Nuclear power has produced nearly 20% of American electricity for decades and has avoided over 1.8 million deaths that would have been caused by air pollution if the same electricity had been generated by fossil fuels [5]. Nuclear technology has also saved millions of lives through the development and use of nuclear medicines, and food irradiation limits the spread of foodborne illnesses and can limit food waste by extending the shelf life of products.

But the nuclear materials used in nuclear energy, like uranium, can also be used in a nuclear weapons program. One of the very first public reports on the potentials of atomic energy, released by a committee of the United Nations approximately one year after the atomic bombings of Hiroshima and Nagasaki, made this connection explicitly [6].



APPENDIX 1: PICTORIAL CHART OF THE PROCESSES USING URANIUM TO PRODUCE ATOMIC ENERGY

A notation accompanying this chart says: "Waste products from the various stages in the processes may be reprocessed to recover the uranium or plutonium which they contain. For simplicity, such operations have not been shown.".

Figure 0.2: This diagram, produced by the newly-formed Atomic Energy Commission of the United Nations in 1946 [6], is likely one of the first nuclear fuel cycle diagrams ever produced. It notes that every step could possibly diverted "to secret weapons production".

By the mid-1960s, five countries had developed nuclear weapons and many more were either pursuing them or considering developing a nuclear weapons program. The U.S. and the Soviet Union led the development of a treaty to limit the further spread of nuclear weapons while explicitly supporting the use of peaceful uses of nuclear technology.

The NPT was a landmark treaty, with several core principles laid out in the individual Articles. Signatories of the treaty were categorized as nuclear-weapon States or non-nuclear-weapon States. The non-nuclear-weapon States agreed not to develop nuclear weapons or other nuclear explosive devices, and nuclear-weapon States agreed not to share their nuclear weapon technology. Everyone agreed to promote and share peaceful nuclear technologies.

And the non-nuclear-weapon States agreed to allow safeguards, defined in the NPT as "verification of the fulfillment of its obligations assumed under this Treaty with a view to preventing diversion of nuclear energy from peaceful uses to nuclear weapons or other nuclear explosive devices."

This mission of safeguards continues today, with over 180 countries as non-nuclear-weapon States signatories of the NPT. While most of the non-nuclear-weapon States have few nuclear materials or facilities, there are hundreds of nuclear reactors and other fuel cycle facilities under safeguards around the world. For example, large nuclear power programs like Canada's and South Korea's have dozens of reactors between them, and there are critical nuclear fuel cycle facilities, like uranium enrichment and fuel fabrication, in Germany and the Netherlands.

All of this verification work, which includes careful evaluation of every nuclear material movement between facilities and inspectors flying around the world to physically assess nuclear materials, must be conducted under a regular budget of about $181.5 million, using the average 2023 EUR-USD exchange rate. This is less than the University of Wisconsin–Madison reported in athletic spending during the 2022-2023 school year.

Figure 0.3: The IAEA regular budget for safeguards is slightly less than the UW–Madison athletic budget.

Given a massive mandate and a limited and stagnant budget, there is a demand for new techniques that help the safeguards process become more efficient while adapting to new facilities and challenges.

My thesis

By the 2000s, work in nuclear fuel cycle simulation had long since diverged from international safeguards. At least informally, the safeguards community perceived that computer codes designed for nuclear fuel cycle simulation were not detailed enough to be useful.

As an early grad student, I started attending conferences on nuclear nonproliferation and introduced myself and my background in nuclear fuel cycle modeling. I was met repeatedly with the perception that the codes that I worked with were not useful and that previous efforts were undereducated in safeguards.

Part of this challenge is the vastly different time scales on which long-term nuclear energy planning and international safeguards operate. The former considers decades, even centuries, into the future and can, therefore, oversimplify what happens on a day-to-day level. The latter is tasked with identifying signs of nuclear material diversion as quickly as possible and is concerned with the patterns of nuclear material movement each day and month.

This skepticism motivated my first project, which was designed specifically to demonstrate how a nuclear fuel cycle simulator could be used within the existing techniques of international safeguards.

Meeting the field of international safeguard where they are

The first project of my dissertation takes an existing methodology developed by the IAEA, acquisition path analysis, and implements it within the ecosystem of a nuclear fuel cycle simulator. This work was meant to show that not only could we use the flexible nature of Cyclus to replicate an existing technique, but that there were opportunities to further advance the technique using specialized capabilities for modeling the movements of nuclear materials that are available within Cyclus.

Acquisition path analysis looks at all parts of the nuclear fuel cycle and simplifies them down to a mathematical model called a graph, where all of the facilities are called nodes, and the nuclear materials that could be traded between them are edges that connect the nodes.

This graph theoretic representation is a very common technique in mathematical modeling. Graphs are used to represent all kinds of systems. A familiar use of graphs is social graphs created by social media. You and your friends on a social media platform can be represented as a graph; each individual person is a node, and the edges represent the connections between you and another person.

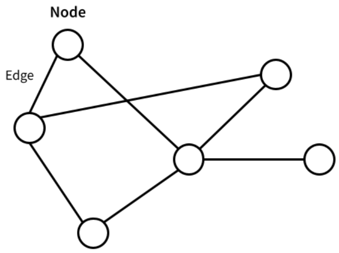


Figure 0.4: A graph

In the most basic type of graph, edges are bidirectional. There's no to or from, both ends of the edge are the same. However, when edges represent nuclear material flows, they are directional. There is a place where the nuclear material comes from and a place where it goes to, like an arrow rather than a line.

A social media graph can go either way. On Facebook, the connections, called "friends", are mutual. Regardless of who sends the request and who accepts it, friendship goes both ways. Platforms that use followers are directional, such as X/Twitter, Bluesky, and Instagram. On these directional graphs, someone you follow is an edge that goes from you to them, and then if that person follows back a second edge goes from that person back to you.

This directional graph, or digraph, is the type of graph that we use to represent the nuclear fuel cycle. After carefully setting up nuclear facilities and nuclear materials that should be in your graph, my tool uses analysis techniques to generate

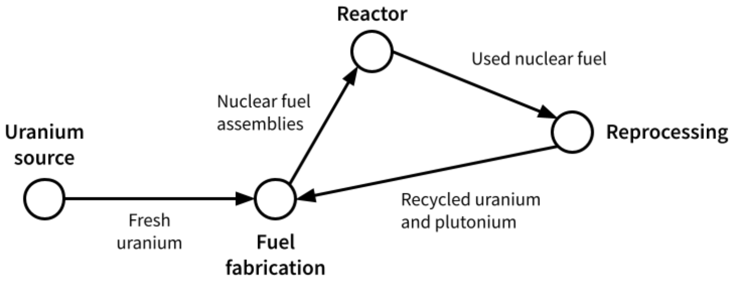


Figure 0.5: A directional graph. If the nodes were people instead of nuclear facilities and the edges were directional follows, this would be a would be a weird love triangle.

several metrics of interest. The famous "Six Degrees of Kevin Bacon" game of acting in Hollywood is an example of a metric from a graph where the nodes are people, and the edges represent the two actors acting in the same movie or show. How many steps connect Kevin Bacon and another actor is a type of metric.

Some of the metrics in my tool include the number of different ways to produce nuclear materials of interest, the shortest path to those materials, and which paths loop back on top of themselves, called cycles.

The tool I created to conduct acquisition path analysis was a great first step to demonstrate a system that could be deployed in an international safeguards context. I presented my work, including a live demonstration of an interactive tool, at the same conference where I had previously experienced skepticism at the usefulness of nuclear fuel cycle simulators. I won first place in the student paper award.

However, I ran into a problem. There wasn't additional information available about where to take my tool next, what new metrics would be helpful to the IAEA. This lack of information would be great for some researchers but not for the highly applied nature of international safeguards.

Consider research in science and engineering as a continuum from basic to applied. I don't mean basic as in simple. I mean basic as in fundamental, studying the core properties of a system. Think about some famous scientists you've heard of, they are all likely people who studied basic science. The intellectual lineage of nuclear engineering is built on the basic science that Marie Curie did to identify the principles of radioactivity and discover the elements radium and polonium.

The other end of the spectrum is typically categorized as engineering, where the basic principles of science are applied to a system to build something or do something with a specific purpose. The field of international safeguards is at the far end of the spectrum on the applied side. The goals are very specific and connect back to the NPT and the mission of the IAEA to promote the spread of peaceful uses of nuclear energy while "supporting global efforts to stop the spread of nuclear weapons".

Any research in international safeguards has a single specific customer: the IAEA. Unlike basic science, research is driven by a clear need, a specific way to apply the new results, technique, or tool being developed. Any new tool or capability must lie within the bounds of the NPT, and all the agreements between individual countries and the IAEA that dictate the details of safeguards implementation.

When I got into international safeguards, I started to hear quips about how university students kept coming up with new ideas, methods, and tools that were novel and warranted a master’s degree or PhD, but they weren’t useful. They didn’t solve any real problems. Or, they could not be applied to a real system because they didn’t understand the needs and limitations of the international safeguards system.

Once I had replicated the technique of acquisition path analysis using the open literature available to me, I ran into a situation where I was concerned that if I went further and came up with something novel I would become another one of those students who did interesting work that was ultimately doomed to live on a shelf, because there was not enough information

available about how to further develop the technique in a meaningful way.

Instead, I wrapped up this tool, called it a prototype, and recognized that I had met my goals. Not only had I replicated the technique within a field cycle simulator, but I had also clearly caught the attention of the community and demonstrated that this type of computational tool, the nuclear fuel cycle simulator, has great promise.

Around this time, I was also given an opportunity to come back to a U.S. National Laboratory, where I had interned before, to work on projects that were already funded by international safeguards, where I could apply my expertise. So, I made a pivot, and I picked up some new work that either became or inspired all of the other parts of my dissertation. I packed up and moved to northern New Mexico to continue my research at LANL.

Refocusing CYCLUS capabilities on the needs of international safeguards

I came to LANL to work on a project to recreate accounting reports for nuclear material, which I believed could be done using the CYCLUS nuclear fuel cycle simulator. These reports are something that all non-nuclear-weapon States must regularly submit with information on their nuclear material, location, composition, and movement.

The IAEA created a format for these accounting reports, and I developed a tool that could take a simulation of a country and create synthetic versions of those nuclear material accounting reports. But while doing that, some limitations of CYCLUS arose. These limitations were critical for international safeguards and had to be addressed.

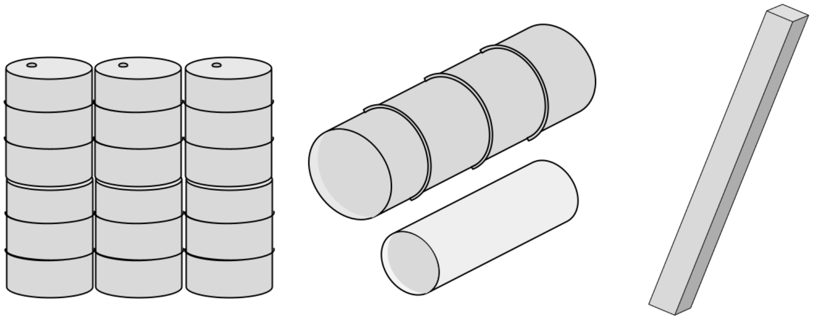
This was reinforced by a meeting I had at the time with somebody who knew how this tool would be applied if it ever got transferred to the IAEA, and her reaction immediately identified some of these deficiencies in our modeling capabilities, pointing out that our tool couldn't be useful if we didn't address these shortcomings. So, I set out to develop several new capabilities that had to be added to the Cyclus software.

Cyclus was designed to be very flexible to enable a wide range of nuclear fuel cycles to be simulated. It comes with a set of "stock" models but also allows users to connect their own nuclear facility models. This is similar to creating and using DLC, or downloadable content, in video games that allows users to expand the world that the game developers created.

My new capabilities specifically target the way that these nuclear facility models interact with the Cyclus core system, which is a market for nuclear materials. In the simplest sense, a facility takes in some type of feed material from another facility and produces some sort of product that it wants another facility to take off its hands. In between those two steps are the chemical and nuclear process models.

Recent research had mostly focused on improving the process models, such as a nuclear reactor model. My own research early on in grad school included being part of a team that created a better uranium enrichment facility model than the stock option. But there had been almost no corresponding improvement in the ways that facilities requested their feed or supplied their products to the rest of the system.

So, I added new inventory management capabilities. In keeping with the ethos of Cyclus, I created a generic set of new capabilities that are flexible and able to be used across many different types of nuclear facilities. Some are simple, like adding the notion of a regular production cycle where facilities are sometimes active and sometimes dormant, simulating a weekend or a clearing or refurbishment period. Some are more complicated, incorporating random numbers or requesting inventory



(a) 55-gallon drums hold uranium ore concentrate after milling

(b) uranium hexafluoride cylinders hold uranium before and after enrichment, in different quantities

(c) A nuclear fuel assembly goes into a reactor to produce power

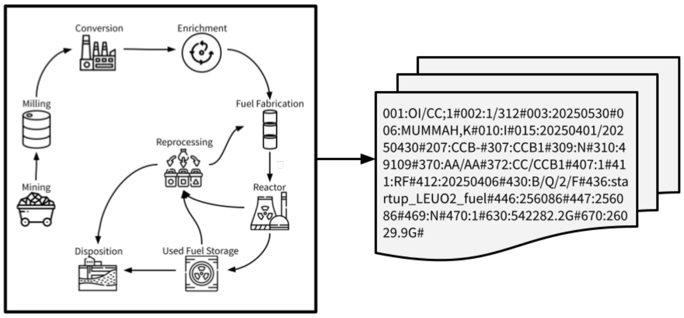
Figure 0.6: Adding packaging capabilities in Cyclus *allows nuclear materials to be represented in realistic quantities, in addition to the realistic chemical compositions they were already modeled as. Here are a few nuclear material packaging types*

in specific amounts, using algorithms similar to ones used to stock goods in a store.

On the product side, I added the notion of nuclear material packaging to Cyclus. In the real world, nuclear materials have very strict international regulations on how and in what quantity they can be moved, and this new capability allows nuclear fuel cycle simulations to capture those patterns.

This work is a story of dozens of small updates to the Cyclus computer code that are each flexible and widely applicable rather than one big flashy new capability. In some ways, that idea is emblematic of my entire dissertation. I set out to identify and fix the deficiencies that were preventing Cyclus from being useful for international safeguards, and it turned out that there were a lot of small things in the way instead of one large project. Research works this way sometimes.

Now that Cyclus simulations include the capabilities needed to produce data for nuclear material accounting reports, the next part of my work creates the capability to generate those reports for any hypothetical set of nuclear facilities over any length of time.



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001:OI/CC;1#002:1/312#003:20250530#0
06:MUMMAH,K#010:I#015:20250401/202
50430#207:CCB-#307:CCB1#309:N#310:4
9109#370:AA/AA#372:CC/CCB1#407:1#41
1:RF#412:20250406#430:B/Q/2/F#436:sta
rtup_LEUO2_fuel#446:256086#447:2560
86#469:N#470:1#630:542282.2G#670:260
29.9G#
```

Figure 0.7: The end result of Code 10 report snippets looks a bit like a small child mashing a keyboard, but it contains everything the IAEA knows about nuclear material movements!

Turning Cyclus simulations into synthetic nuclear material accounting reports

One of the requirements for non-nuclear-weapon States is to submit information about the location, composition, and movement of all nuclear material in their country. The system for how to do this was developed decades ago around punch cards. While our computer systems have evolved significantly in the intervening years, the format for submitting nuclear material accounting reports remains linked to the style of punch cards. This system is typically called Code 10, because it is described in the tenth part of the model agreement that countries arrange with the IAEA.

Real nuclear material accounting reports are in the Code 10 format, so replicating this information synthetically using computer simulations should be in the same format, too. Models trained on synthetic data could relatively easily be used on real data, and using this format ensures that only the information contained in real reports is incorporated into the synthetic reports.

Cyclus generates a lot of information that doesn't end up in nuclear material accounting reports. For example, some of the internal movements in a facility are simulated in Cyclus but do not count as “inventory changes” under the purview of Code 10. If I trained a model to look for signs of nuclear material diversion using the entire Cyclus simulation, I would capture this excess data that the IAEA does not have for real countries, which is undesirable.

Converting a Cyclus simulation into Code 10 format reports is a bit like translating between two languages. Some of the information has a very straightforward translation, such as time. Others require new context, such as converting the individual processes of a nuclear fuel cycle into the regions of importance to safeguards, called material balance areas.

Finally, some ideas only exist in one “language” or another. Cyclus simulates nuclear materials as masses, but some entries in the Code 10 reports are based on volume. The conversion from mass to volume can be straightforward. If you remember back to high school science class, density is mass divided by volume. Rearranging this equation results in volume equals mass divided by density. However, density is not a concept that exists in Cyclus, so some special handling is required to overcome this limitation. This is one way where the new nuclear material packaging capability from the previous section comes in handy. Nuclear material packages have a specific mass and a specific volume (implying a specific density), and therefore, when nuclear materials are shipped between facilities using these packages, it is possible to know their volume.

With this new tool, it is now possible to simulate the movement of nuclear material from mining to disposal for an entire country over the course of decades and then see what nuclear material accounting reports should look like for that entire period. The final step of this work is to create realistic but fake countries to demonstrate all these new capabilities together.

Creating realistic but fictitious countries

Computer modeling frequently creates worlds that do not exist. Often, this is some possible near future, something that could happen to a real system if it evolved in a certain way. This is very common in nuclear fuel cycle modeling; if you want to see how a fleet of nuclear waste-burning reactors would work, it makes sense to start from a real country that already has nuclear reactors.

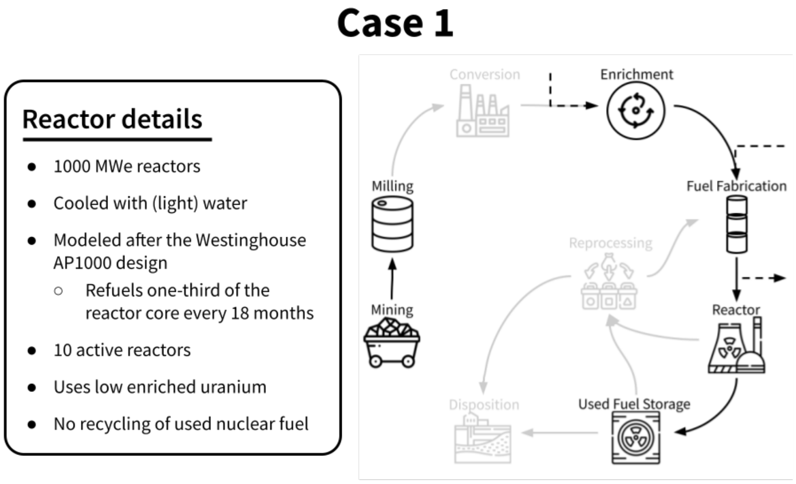
In some cases, though, it doesn't make sense to start from a real country. Real countries are complicated, and the details may not be publicly available. Existing nuclear fuel cycles may not be a good proxy for "nuclear newcomer" countries that are building their nuclear power system from scratch in the 2020s and beyond rather than the 1960s and 1970s. And in the case of international safeguards, real countries are political. Using a real country for a demonstration, even with innocuous intentions, could accidentally make a political statement about which countries "should" be considered as possible proliferators.

Researchers often come up with one-off fictitious countries to use in their work. My team at LANL did this for a project report. A PhD is a chance to do research in a more robust way, however, so I decided to develop a methodology to comprehensively describe a nuclear fuel cycle and then generate a set of fictitious countries.

I built on a 2014 study for the U.S. Department of Energy, called the *Nuclear Fuel Cycle Evaluation and Screening – Final Report* (E&S) study, that aimed to describe nuclear fuel cycles using six specific parameters, but did not attempt to build entire fictitious countries. I found that I needed to expand to fifteen parameters to more comprehensively describe the nuclear reactor system, the type of fuel recycling used, and the other facilities in the fuel cycle.

Then, I got to work using my parameters to build a set of thirteen fictitious countries, which I call cases. These are, obviously, not a comprehensive list of possible fuel cycles. The E&S study produced almost 4,400 reactor systems and was able to group them into 40 similar categories. With all the extra parameters I added, it would not be useful or feasible to enumerate all the possible permutations, even after getting rid of options that would not be possible due to physics.

Instead, I carefully constructed the fake countries such that all the options for each parameter were used in at least one fake country. Consider one of my parameters, reactor power. Reactors are categorized as micro, small, medium, or large, depending on the amount of power they produce. At least one fake country has a reactor at every power level. The smallest design, in Case 4, uses microreactors that produce only 2 megawatts of electricity, or about the same as a single modern wind turbine. The largest in Case 10 produces over 1300 megawatts, which at the typical capacity for a nuclear power plant would produce the same amount of annual electricity as is consumed in the state of New Hampshire [7].


Case 1

Reactor details

- 1000 MWe reactors
- Cooled with (light) water
- Modeled after the Westinghouse AP1000 design
    - Refuels one-third of the reactor core every 18 months
- 10 active reactors
- Uses low enriched uranium
- No recycling of used nuclear fuel

Figure 0.8: This is some of the information associated with each of my fictitious countries. The reactors are defined in enough detail that they can be modeled in similar computer codes, and the nuclear fuel cycle includes information on which facilities exist within the country (materials from the missing facilities have to be imported from another country).

Conclusions

The final step of my research was to demonstrate the types of analyses that people could do with the new capabilities I developed. Eventually this work might be used to look for subtle patterns that could indicate nefarious actions, but first I needed to show how we could model and then analyze benign disruptions to the system. I showed how future users could run many iterations of simulations with slight changes and evaluate what, if any, effects are detectable elsewhere.

Until now, no one has claimed to be able to generate an entire country's worth of synthetic nuclear material accounting reports. This represents a significant new capability that can open new doors in the fields of nuclear fuel cycle modeling and international safeguards.

In an ideal world, someone with all the information about a country's nuclear fuel cycle (real or fictitious) would use my tools to generate millions of plausible nuclear material accounting reports. This information could be used to look for novel signatures of bad behavior, like nuclear material diversion, and to test how new nuclear facilities would fit into the safeguards structure. This work requires fuel cycle expertise and a significant amount of data science (including machine learning) expertise to parse the generated data. Although it was out of the scope of my PhD work, I hope that it can eventually happen.

1 MOTIVATION

The 1970 Treaty on the Non-Proliferation of Nuclear Weapons (NPT) [3] is the cornerstone of global efforts to limit the spread of nuclear weapons and work towards disarmament of nuclear explosive devices, while allowing and promoting the peaceful uses of nuclear technology. It is the role of the International Atomic Energy Agency (IAEA), an "autonomous international organization within the United Nations system" [8, 9] to verify parties' compliance to the NPT.

The IAEA 2024 Regular Budget for nuclear verification, or international safeguards, was €167.7 million [10]. Using the average 2023 EUR-USD exchange rate, this is about $181.5 million, about $12 million less than the University of Wisconsin–Madison spent on athletics in the 2022-2023 school year[1] [12]. The work covered by the Regular Budget includes verifying the correctness and completeness of State accountancy reports and Additional Protocol declarations in over 170 countries to confirm nuclear materials are not being used to develop nuclear explosive devices. This is to say, a single university in the United States[2] has more money to spend on their athletic programs than the IAEA has to verify that nuclear materials remain strictly in peaceful uses in nuclear facilities across the world. Improvements in the effectiveness of international safeguards while maintaining or even increasing objectivity and reproducibility are of high value to the nonproliferation community.

IAEA analyst and inspector time are already strained, with a budget that has been and will likely continue to be stagnant in the near future [13, 14].

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[1] The last year currently available. Expenses from the University annual report to the NCAA, which differs from the University's internal financial expense structure, which was reported as $167 million [11].

[2] According to the Knight-Newhouse College Athletics Database, UW–Madison reported the 10th highest spending on athletics in 2022-23. The highest single spender, the Ohio State University, had over 40% higher expenses for their athletic programs than the IAEA 2024 Regular Budget for nuclear verification.

Many “nuclear newcomer" countries are considering developing nuclear power programs for the first time, and others are working on expanding their nuclear facilities with small modular reactors (SMRs) or advanced reactors with very different designs than the large (gigawatt-scale) light water reactors (LWRs) that currently dominate the global market. At this inflection point, it is even more critical for the international safeguards community to streamline and enhance the safeguards process.

The goal of this dissertation is to enable State-level nuclear fuel cycle simulations and analyses that could be used to advance the safeguards implementation process. Decades ago, nuclear fuel cycle simulators had been evaluated and considered to be of marginal use to the international safeguards community because of limited simulation fidelity. Since that time, capabilities of nuclear fuel cycle simulators have advanced considerably. The first step of this work was to explore whether the nuclear fuel cycle simulator Cyclus can be used to conduct an existing methodology in use for safeguards, acquisition path analysis (APA).

Chapter 3 demonstrates how any simulation that can be defined using agents within the Cyclus ecosystem can be used to conduct the core methods of APA, and can be coupled with the information available from a fuel cycle simulation to further consider the possible nuclear material flows, given the set of nuclear fuel cycle facilities and technical capabilities of a State. The rest of this dissertation builds a capability to generate synthetic nuclear material accounting reports on the scale of an entire State.

Nuclear material accounting reports are one of the core pillars of international safeguards. States[3] who have concluded a comprehensive safeguards agreement

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[3] The IAEA refers to nations as States, traditionally capitalized. For both real and fictitious countries used in this dissertation, the same style is used.

(CSA) with the IAEA (see Chapter 2.2) must keep track of the location, composition, and movements of their nuclear materials and submit this information to the IAEA on a regular basis for evaluation.

Because these reports play such a crucial role in the safeguards process, the ability to generate synthetic reports for any existing or future State can be useful for planning and research purposes. For nuclear technologies that are not yet commercialized, such as fluid-fueled Molten Salt Reactors (MSRs), or countries who are planning large additions to their nuclear fuel cycle in the upcoming years, these reports could be used to prepare for the future. Synthetic reports could be used to develop analysis techniques before needing to apply them to real facilities, real stakes. This work could inform safeguards by design (SBD), where the requirements of a safeguards system, including nuclear material accounting structures and reporting requirements, are incorporated into the design and planning stage of a nuclear facility instead of applied retroactively, which has been the case for most facilities under safeguards. A tool to systematically generate synthetic reports could be used to efficiently test possible accounting structures.

The ability to generate synthetic nuclear material accounting reports can also be used to study the impact of disruptions, benign or nefarious, on a fuel cycle by systematically generating a large volume of simulations and evaluating the impact on accounting reports.

Until now, none of these applications would be plausible because no tools were available to generate nuclear material accounting reports in the exact style and format that States submit their reports to the IAEA, colloquially called Code 10. Chapter 5 describes the development of a tool to convert Cyclus fuel cycle simulation outputs into accounting reports, specifically inventory change reports (ICRs).

While Cyclus is well-suited to generate the scope of information needed to create nuclear material accounting reports by its modeling of the movements of nuclear materials throughout the cradle-to-grave nuclear fuel cycle, the Code 10 tool required additional capabilities for simulations to reach the required spatial and temporal fidelities necessary in international safeguards.

Cyclus and other nuclear fuel cycle simulators have mostly been developed and used for long-term nuclear energy planning, which allows for long time steps of a month or more, with nuclear material movements aggregated accordingly. Because long time steps are acceptable for simulations running decades or centuries, nuclear material movements internal to facilities are not of high interest. Conversely for safeguards, simulations must have one-day time steps because inventory changes must be recorded on the day in which they occur, and nuclear material accounting structures are based on material balance areas (MBAs) and key measurement points (KMPs), of which there can be multiple within a nuclear facility.

Recent work by other Cyclus developers has focused on increasing the simulation fidelity for individual facility models such as reactors, enrichment and pyroprocessing (reprocessing) [15, 16, 17]. However, the entire system lacked capabilities to model realistic patterns of nuclear material movement between facilities and MBAs, which are core to nuclear material accounting reports.

Nuclear materials have historically been modeled as a single bulk mass moved during each time step, such as the entire mass of a batch of nuclear material as a single item. However, nuclear material accounting requires individual items, such as fuel assemblies or UF_6 cylinders.

Chapter 4 introduces novel systematic and stochastic behavior patterns on the receiver and shipper ends of transactions into the Cyclus Toolkit, which allows them to be implemented in any agent developed for the Cyclus ecosystem and, therefore, any simulation. Packaging capabilities were added to Cyclus to allow any resource to have a packaging type and mass restrictions based on the way it is packaged. These new patterns and packages can be applied across every step of the nuclear fuel cycle. A new paradigm is also introduced for developing simulations with the spatial fidelity required for nuclear material accounting, which relies on the MBA as the fundamental unit of space, rather than the facility.

With these new modeling capabilities allowing State-scale nuclear fuel cycle simulations to generate information about nuclear material movements and compositions, Chapter 5 details the development of a tool to convert those simulation outputs into the exact style and format that States with concluded CSAs must submit regularly to the IAEA.

Recognizing the need to demonstrate all of these capabilities at the scale of an entire country, Chapter 6 includes a set of country-sized but synthetic nuclear fuel cycles. This avoids the need to inadvertently imply that any real country might be a particularly-useful example State to investigate from an international safeguards perspective. Prior work, including by this author, has typically built one or two special-purpose fictitious States in order to demonstrate new functionality, with the example discarded soon after. The fictitious State cases in Chapter 6.4 were designed to replicate a broad scope of fuel cycles, with a few similar to the no-recycling LWR and heavy water reactor (HWR) fuel cycles that are most common across the world and also possible future fuel cycles that a State could plausibly implement in the coming decades. They were designed to be reused and with enough specificity to be replicated in other fuel cycle simulators .

Instead of reinventing the wheel, case-development work leveraged the results of the *Nuclear Fuel Cycle Evaluation and Screening – Final Report* (E&S) study that was published by a collaboration across the U.S. national labs in 2014 as the foundation for which reactor systems could offer benefits and present challenges to implement in the future. However, the E&S report did not consider many fuel cycle factors such as reactor power and cycle lengths, or State-wide factors such as total power and in-State fuel cycle facilities.

Chapter 6 systematically evaluates the parameters needed to describe a State's fuel cycle, starting with and expanding beyond the E&S study's seven parameters. Thirteen separate fictitious States, called cases, were developed in order to cover a wide breadth of possible nuclear fuel cycles.

Finally, Chapter 7 uses a subset of the fictitious state cases from Chapter 6.4 to demonstrate how the new behavioral capabilities can be incorporated into full scale simulations and used to produce synthetic nuclear material accounting reports for an entire country.

To date, there have not been any other efforts identified that attempt to use cradle-to-grave nuclear fuel cycle simulations to recreate a set of regular accountancy reports in line with the complexity and document forms that States send to the IAEA. Therefore, generating realistic state accountancy reports is a novel and valuable addition to existing system-scale nuclear fuel cycle simulation.

The development of case studies designed to capture a breadth of nuclear fuel cycle possibilities without direct connection to current States or quick-to-change future plans also holds value for the broader nuclear fuel cycle community. As described in Chapter 6, these case studies can enable future benchmarking of tools without creating novel case studies from scratch, building on prior literature rather than reinventing the wheel. This work will also feed back into safeguards work by providing a standardized set of wide-ranging test cases to demonstrate software capabilities.

2 LITERATURE REVIEW

2.1 System-scale nuclear fuel cycle simulation

The lifecycle of uranium and other nuclear materials is an interdependent system that has been studied since the advent of the atomic age [6]. Early uses of uranium, in both nuclear weapons and nuclear energy, were developed and controlled by State actors, i.e., countries managing most or all the steps in the fuel cycle. This vertical integration enabled full control of construction, operation, and, ultimately, the production rate of nuclear commodities from cradle to grave.

Modern nuclear energy systems comprise a decidedly more complex set of public, private, and government corporations and regulators. While some countries maintain a high level of State control over their nuclear fuel cycles, like France and Russia, they still transact nuclear material in the form of imports and exports to other nations. Other countries, such as the United States, do not have State control over most of their fuel cycle[1], leaving a patchwork of domestic and international corporations to decide when to research, design, construct, operate, retire, and eventually dismantle and dispose of nuclear materials and facilities.

To assess these systems and study potential futures, nuclear fuel cycle simulators were developed. Nuclear fuel cycle simulators are computational tools designed to track nuclear materials' presence, quantity, and characteristics as they move between or within nuclear facilities.

They range in capability and open access depending on their developer and intended purpose. Most fuel cycle simulation tools are proprietary, such as the

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[1] Geologic disposal of used nuclear fuel is a notable exception. Under the Nuclear Waste Policy Act, as amended, the U.S. Department of Energy is responsible for siting, obtaining a license, constructing, and operating a geologic disposal facility for commercial used nuclear fuel (UNF)

French Commissariat à l'Énergie Atomique et aux Énergies Alternatives (CEA)'s COSI [18, 19], and UK National Nuclear Laboratory (NNL)'s ORION [20]. Several nuclear fuel cycle simulators have been primarily developed at universities, which typically allow for greater ease of access to researchers but are more likely to suffer from a lack of consistent funding for maintenance. These include Massachusetts Institute of Technology (MIT)'s CAFCA [21], University of Texas at Austin's VEGAS [22], and the University of Wisconsin's Cyclus [23, 24]. At the highest ease of access are free and open-source software (FOSS) tools, which are available to anyone for free and have a public code base. As of early 2024, Cyclus and CLASS [25], the French collaboration between Centre national de la recherche scientifique (CNRS) and Institut de radioprotection et de sûreté nucléaire (IRSN), were the only two known FOSS nuclear fuel cycle simulators. The University of Wisconsin has developed a CLASS reactor model for Cyclus called cyCLASS, bridging the two FOSS fuel cycle simulators.

In part due to its accessibility compared to similar tools, Cyclus has found active use and/or development across several institutions over the last decade. Some of the recent university developers and analysts of Cyclus include the University of Illinois at Urbana-Champaign [26, 27], Princeton University [28], and RWTH Aachen University (Germany) [29, 30]. Several national laboratories are also Cyclus users, although they are less likely to open-source their models and analysis. Recent lab users include Los Alamos National Laboratory (LANL) [31], Argonne National Laboratory (ANL) [32, 33], Oak Ridge National Laboratory (ORNL) [34], and Pacific Northwest National Lab (PNNL) [35, 36].

2.1.1 Agent-based models

Cyclus is an agent-based model (ABM). Sometimes referred to as individual-based modeling (IBM) in fields such as ecology, ABMs are a way of representing a real system as a set of individual actors. In a simulation, these individual actors, called agents, act autonomously with individual underlying logical patterns as they interact with their environment. ABMs have been used in many different fields, from predator-prey population models in ecology to pedestrian dynamics for urban planning [37], and to estimate the spread of SARS-CoV-2, the coronavirus that causes COVID-19 [38].

Agents in Cyclus represent individual processes or facilities in the nuclear fuel cycle. Agents interact by exchanging commodities, which represent nuclear materials. Cyclus represents the passage of time in discrete, fixed time steps. Users set the time step length in seconds for each simulation, but it is typically one day (86,400 seconds) for high-fidelity nonproliferation-focused applications, or one average month (2,629,800 seconds) for simulations that span decades, or more than a century for long-term nuclear energy planning. See Appendix A for a detailed description of Cyclus terminology as it pertains to this work.

Some nuclear fuel cycle simulators, like the International Atomic Energy Agency (IAEA)'s Nuclear Fuel Cycle Simulation System (NFCSS) [39], model nuclear reactors as an aggregated fleet. Typically equivalent to modeling a single mega-reactor based on the sum of all reactors it is based on, this is a very low-fidelity way to represent the fuel cycle. It results in unrealistic movement patterns, especially for large countries where the actions of dozens of reactors are stuffed into one process. NFCSS cannot model nuclear materials individually, and when demand is higher than supply can produce unphysical negative quantities. Because reactors are modeled as a fleet, there is no way to study nuclear material movements into or out of a specific reactor, or to inject disruptions that affect a single reactor. The capability to model facilities as individual actors in an ABM are especially important to the application of nuclear fuel cycle simulators to nonproliferation, where a single facility acting differently can be a sign of disruption or nefarious action.

2.1.2 Fuel cycle case studies

Nuclear fuel cycle simulators have traditionally been used to support a nuclear energy system, either by optimizing material usage in current facilities [40] or by creating/studying future transitions to a system with a different quantity of reactors and/or different reactor designs [41, 42, 43]. Several studies have benchmarked nuclear fuel cycle simulator performance, such as a validation study [44] comparing the simulators used across four U.S. national laboratories, DYMOND [45], VISION [46], ORION [20], and MARKAL [47], as well as more recent efforts [48, 49], including several that have included CYCLUS [50, 51].

Developing nuclear fuel cycle simulator capabilities for nonproliferation applications, long recognized as a valuable potential use case of these tools [23], creates additional challenges with regard to modeling decisions. Using a fuel cycle simulator for long-term planning typically does not require modeling with high temporal or spatial fidelity as using the same tools for nonproliferation and international safeguards purposes does.

In 2014, the Office of Nuclear Energy within the U.S. Department of Energy (DOE) published a report from a multi-year effort to characterize equilibrium fuel cycles and the benefits they may offer to the existing U.S. fuel cycle of once-through light water reactors [1]. This extensive report, the *Nuclear Fuel Cycle Evaluation and*

Screening – Final Report (E&S), provides a useful foundation for the metrics needed to characterize a fuel cycle. Table 2.1 summarizes the primary features considered in the study. The work implies the availability of fuel cycle services but does not consider fuel cycle capabilities in their parameter scope.

Table 2.1: Summary of primary features, sometimes called discriminators, in the E&S study [1]

FCO Discriminator	Options
Recycle	Once-through, recycle (limited), recycle (continuous)
Recycled elements	U, Pu, Th, transuranics (TRU)
Criticality	Critical, sub-critical
Neutron spectrum	Thermal, fast (including intermediate)
Feed fuel	Uranium, uranium-thorium, thorium
Enrichment	Required, no/not applicable
Stages	1 stage, 2+ stages

Several years after the E&S study was published, a collaboration between five U.S. national laboratories led by Nicholas Brown identified the features and capabilities needed to test a wide range of capabilities required and desirable of an effective nuclear fuel cycle simulator. The work also benchmarked the many tools created in the United States and across the world [52]. The specific focus of the paper was centered around transition studies, which include the temporal component of moving from one type of fuel cycle (typically GW-scale light water reactors (LWRs)) to another over the course of decades.

The conclusion reached by Brown *et al.* was that concrete scenario development was needed to expand beyond their basic set of criteria, although this was not attempted at the time. No follow-up studies have been identified that have addressed this call for future work.

2.2 International Safeguards

Since it entered into force in 1970, the Treaty on the Non-Proliferation of Nuclear Weapons (NPT) has been the legal core of intergovernmental efforts to limit the spread of nuclear weapons. Under Article III of the Treaty on the Non-Proliferation of Nuclear Weapons (NPT), the International Atomic Energy Agency is tasked with implementing safeguards to verify that non-nuclear-weapon States (NNWS) are not diverting material from peaceful uses towards a program to produce a nuclear explosive device.

According to their Annual Report [53], in 2023 the IAEA drew safeguards conclusions for 189 States, including each of the five nuclear-weapon State (NWS) recognized by the NPT. Safeguards conclusions are an annual formal declaration by the IAEA about the condition of safeguards implementation for each State in the previous year. The conclusions that can be drawn depend on the State's safeguards agreement in force. For all agreements, the IAEA may choose to draw no safeguards conclusions. See Appendix B for more details on safeguards terminology, including conclusions.

Drawing safeguards conclusions requires a substantial effort of Agency time and resources. Given the expanding amounts and sources of data available without a corresponding rise in inspectors and analysts, techniques that can reduce analyst workload are of high value.

2.2.1 Nuclear Material Accounting at the State Level

All non-nuclear-weapon State (NNWS) Parties to the NPT must conclude, or agree upon, a comprehensive safeguards agreement with the IAEA on the basis of a template document, INFCIRC/153 (corrected) [54]. These agreements become public, as information circulars (INFCIRCs) that are available on the IAEA website.

In addition to the comprehensive safeguards agreement (CSA), States must develop Subsidiary Arrangements [55] that specify additional details about safeguards implementation within a given State, including the development of a State system of accounting for and control of nuclear material (SSAC) by which nuclear material accounting is conducted and reported to the IAEA. Unlike CSAs, none of the information agreed upon in Subsidiary Arrangements becomes available to the public unless a State chooses to publish it.

Subsidiary Arrangements have a general part that applies to the entire State, and Facility Attachments (FAs) that specify the exact details of implementations for all facilities and locations outside facilities (LOF) in the State.

FAs contain detailed information about a facility's design, safeguards measures, and accountancy. They include the precise breakdown of material balance areas (MBAs) and key measurement points (KMPs) for the facility, as well as the expected types of inventory changes to occur in the facility, and therefore factor heavily into how materials and their movements are recorded in accounting. Model FAs are often the basis or starting point for an agreement and propose MBAs and KMPs. However, these documents are not widely available to the general Research and Development (R&D) community.

While there is not a "one size fits all" process to succinctly describe all possible accounting structures, this work follows the nuclear material accounting concepts and reporting structure recommended in the IAEA's *Safeguards Implementation Practices Guide on Provision of Information to the IAEA* (IAEA Services Series 33) [56] and in the Model Subsidiary Arrangements. Most notably, the 10th section, "Code 10 Contents, Format and Structure of Reports to the Agency," shortened as Code 10, details the reporting structure developed by the Agency [57].

Two more safeguards agreements may be optionally adopted by a NNWS and the IAEA, a small quantities protocol (SQP), and an Additional Protocol (AP). An SQP is an agreement that minimizes the burden of implementing the CSA for states with “little or no nuclear activities” [58]. The AP is an agreement on the basis of INFCIRC/540 [59] that strengthens safeguards by adding new tools to the IAEA, such as environmental sampling at suspected undeclared locations and complimentary access inspections to “resolve a question or an inconsistency relating to correctness and completeness of the information provided by a State...” [60]. These agreements, along with agreements concluded by NWS, called voluntary offer agreements (VOA), and agreements with States that are not Party to the NPT, called item-specific safeguards agreements, are beyond the scope of this work and do not affect the structure of regular accounting reports.

MBAs and KMPs are the spatial unit used to account for nuclear material. When accountancy reports and State declarations (if the Additional Protocol is in force) are submitted, they are submitted on a per-MBA basis. The precise definitions of facilities, MBAs, KMPs, and LOFs are agreed upon in Subsidiary Arrangements between a State and the IAEA, but this work will define a set of notional MBAs across the nuclear fuel cycle.

2.2.2 Code 10

Three types of nuclear material accounting reports must be submitted to the IAEA for each MBA in a State. As summarized by the IAEA Safeguards Implementation Practices (SIP) guide [56],

> **Inventory change reports (ICRs)** provide information about changes in the inventory of nuclear material (including transfers within a State from

one MBA to another) and are submitted as specified in the Subsidiary Arrangements (typically within 30 days after the end of the month in which the changes occurred or were established).

Material balance reports (MBRs) provides a summary of the material balance in the MBA, reflecting all inventory changes in a material balance period (MBP). MBRs are submitted as specified in the Subsidiary Arrangements (typically, within 30 days of a physical inventory taking (PIT)).

Physical inventory listings (PILs) include all batches of nuclear material separately and specify material identification and batch data for each batch at each KMP. PILs are submitted with the corresponding MBR (except for an initial PIL, which is a standalone report).

This work follows the Code 10 reporting structure that States must use to submit their accounting reports to the Agency [57].

There are three versions of Code 10 that States may choose from when deciding how to submit their regular accounting reports to the IAEA. Labeled format, fixed format, and, more recently, XML format all contain the same information, each presented slightly differently.

2.2.3 Synthetic State accounting data

Information about a State's inventory and movements of nuclear material is highly sensitive, both from a commercial perspective and from a security perspective. States (and commercial entities) do not publish this information, and the IAEA – who receive detailed information from States as accounting reports – considers all information about nuclear materials location and composition Safeguards Confidential [61, 62]. Even within the Agency, information marked as Safeguards Confidential can only be accessed by those who have a direct need to analyze and summarize the information for that particular State.

For this reason, there have been few attempts to capture and study the big picture of nuclear materials on the State level. Previous safeguards research efforts using both Cyclus and other tools have focused on improving fidelity at the level of an individual facility or even a single process.

One current effort by the IAEA has attempted to anonymize real data for a single type of facility for use as a test bed for new data analysis techniques. Using only data from nondestructive assay (NDA) and destructive analysis (DA) taken by inspectors in real facilities, a classification and regression tree (CART) model was trained to generate synthetic data for an enrichment plant [63]. However, this effort focuses on a different data stream, safeguards inspector-generated information rather than State accounting reports, and again considers only a narrow slice of the fuel cycle. Because the IAEA has access to real data, much of the effort was to ensure that the CART model generates a realistic but truly synthetic data set that cannot be used to trace information back to a real facility, as there are only a small number of enrichment plants around the world. That research has not yet produced a publicly available data set, and it is currently unclear if this data set will ever be made available outside the Agency rather than remaining for internal use.

The IAEA is also not an R&D organization. It is not in their mission to always push at the forefront of innovation with a large research workforce, and their current budget could not support the cost and human capital of highly experimental R&D anyway. Many of the tools and techniques deployed by the Agency are developed at government laboratories and universities and only then transferred to the Agency at a high technology readiness level for active use by analysts and safeguards inspectors [64, 65]. When the Agency accepts a technology transfer, it must be ready for use in the field, in inspections at nuclear facilities, and in actual safeguards assessments.

Therefore, a large literature gap exists in analyzing an entire State's nuclear material information. No real data is available to researchers, and fuel cycle simulations have either focused on very high fidelity for one facility or very low fidelity (one month or longer time steps) for long-term nuclear energy planning.

2.2.4 State Level Concept and Acquisition Pathway Analysis

The State-Level Concept (SLC) is a notion that a State's entire nuclear fuel cycle, including facilities, nuclear materials, and technical capabilities, should be considered holistically when applying international safeguards [66, 67]. While simple in concept, enacting the SLC in practice has been a decades-long effort by the IAEA and organizations that provide research and technology to the international safeguards regime [68].

Early safeguards efforts developed from the 1970 NPT focused on verifying nuclear material declarations at individual declared facilities, which presented enough of a challenge with the rapidly growing and changing industry. Safeguards were developed for a type of facility, such as on-load or off-load reactor, and then all facilities of that type were treated identically. This made sense at the time given the significant reliance on expert judgment needed to develop safeguards approaches in the early days. This meant that every nuclear facility in every country was treated as an independent unit. Two identical facilities in two countries would be treated the same without regard to other factors, such as the existence or technical capability to conduct other processes within the nuclear fuel cycle. After multiple States were found to be in noncompliance with the NPT and the IAEA failed to identify these breaches in a timely manner, the international safeguards regime was revised to ensure that the IAEA had the tools, information, and access necessary to detect undeclared or covert nuclear activity [69]. This principle is reflected in the phrase "correct and complete," which reflects the importance of not only verifying that a State's declarations are correct but also that no facilities or processes were withheld as they had (or may have) been, for example in Iraq in the 1990s [70] and in the Democratic People's Republic of Korea [71].

In the mid-1990s, the process of applying safeguards on an individual facility basis was re-examined [61]. The modern approach to safeguards, or the SLC, is intended to consider the entire set of nuclear facilities and technical capabilities that exist within a State when determining safeguards and ensuring that a State's declaration is both correct and complete [66]. When the SLC is applied to a particular State, the safeguards implementation unique to that State is called a State-Level Approach (SLA). However, it can be complicated to consider an entire State in a rigorous technical and objective manner without political considerations or the perception thereof.

Several countries have raised concerns with the SLC, most notably Russia in June 2012, arguing that the approach could be subjective and perhaps discriminatory [72]. This, along with concerns raised by other States, has prompted the IAEA and the larger international safeguards community to prioritize creating SLAs in a manner that is as transparent and objective as possible [73].

As the IAEA began to consider the entirety of a State with regard to nuclear safeguards, extensive documentation of nuclear facilities led to the notion of enumerating and evaluating the full scope of possible material movements that could plausibly result in the creation of material suitable for use in a nuclear explosive device. The term *acquisition pathway* appeared around the time that the IAEA began implementing State-level safeguards, rather than at the facility-level [74].

Around this time, the IAEA developed an internal set of documents called the Physical Model, which comprehensively identifies and describes the set of facilities that the IAEA safeguards [75]. Along with the development of the Physical Model, summarized in Figure 2.1, the IAEA developed a generic set of material movements between these facilities, which they called the acquisition path.

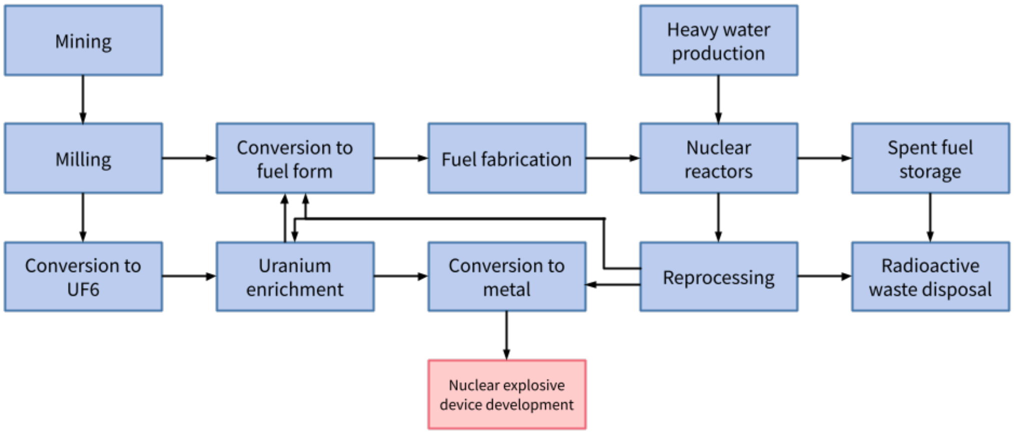

Figure 2.1: Basic elements of the IAEA Physical Model

Some prior work exists in improving methods of conducting acquisition path analysis (APA). Early published iterations relied heavily on expert judgment and have limited automation, including work published by LANL [76, 77] and a case study by the IAEA [78].

More recently, a special-purpose tool was developed by LANL. The tool is not publicly available, and little has been published in open literature [79]. While the tool automates aspects of APA, it models all steps of the fuel cycle as fleets (see Section 2.1.1), not as individual agents. The tool also uses a generic time assessment for how long it would take for an acquisition path step to produce a significant quantity (SQ) of material, the "approximate amount of nuclear material for which the possibility of manufacturing a nuclear explosive device cannot be excluded" according to the IAEA Safeguards Glossary [2]. The SQ values, given in Table 2.2, are commonly used in safeguards analyses and in developing safeguard implementation approaches. Plutonium with ^{238}Pu content above 80% is the only material not assigned a significant quantity, and is exempted from the IAEA's definition of a special fissionable material [2].

There is an opportunity to use Cyclus's capabilities for individual facility modeling and material flows to conduct a more detailed APA.

Table 2.2: Significant quantity values by element and isotopic composition [2]

Element	Isotopics (wt%)	Use	Significant Quantity
U	$^{235}U \geqslant 20\%$	Direct-use	25 kg
U	$0.7\% < {}^{235}U < 20\%$	Indirect-use	75 kg
U	$^{235}U = 0.7\%$	Indirect-use	10 tons
U	$^{235}U < 0.7\%$	Indirect-use	20 tons
U	$^{233}U > 0\%$	Direct-use	8 kg
Pu	$^{238}Pu < 80\%$	Direct-use	8 kg
Pu	$^{238}Pu \geqslant 80\%$	None	None
Th		Indirect-use	20 tons

2.3 Fuel cycle modeling as applied to nonproliferation and international safeguards

There have been several previous efforts to create specific tools or modify existing nuclear fuel cycle simulation tools to be more useful to the nonproliferation and international safeguards communities. These efforts have mainly focused on the facility-level, rather than State-level. These have included developing new facility models, called archetypes, that include desirable behaviors such as integrated safeguards, and have primarily focused on two sensitive stages of the nuclear fuel cycle, namely uranium enrichment and reprocessing.

2.3.1 Nonproliferation efforts in CYCLUS

The first set of enrichment models created for the CYCLUS ecosystem was developed as part of CYCAMORE, a set of archetypes designed by the CYCLUS team [80]. They were based on a generic separative work unit (SWU) calculation with conservation of mass and assuming no holdup. However, relying on SWU calculations misses any granularity of designing and operating a cascade of gas centrifuges and is, for example, unsuitable for studying the behavior of cascades when they are off-normal operational states.

A more detailed centrifuge model was developed by Meghan McGarry at the University of Wisconsin–Madison in part to address these challenges [16]. These models were then expanded and used to study potential behavior post-Joint Comprehensive Plan of Action (JCPOA), colloquially the "Iran nuclear deal", by Mouginot, Stomps, and this author [81].

Most prior efforts to simulate safeguards measurements have either used the simulation as a direct ground truth measurement or implemented simulated process measurements in post-processing after the simulation had been completed. To date, there have been two efforts known to have integrated some notion of safeguards activities into CYCLUS archetypes. One facility archetype in the mbmore packages developed by McGarry is RandomEnrich, which includes "inspector swipes" as an integrated safeguards feature [82]. The user defines a maximum number of time steps between inspections, with inspections occurring between 1 and the maximum (inclusive) time steps, a fixed number of swipes to be taken during each inspection, and both false positive and false negative likelihoods if desired.

The other is a pyroprocessing archetype called PyRe, developed by Westphal as part of his Master's work at the University of Illinois [17, 83]. PyRe implemented a unique diverter class to modify facility parameters to produce the desired product outside of declared operations. Westphal's thesis demonstrates the depth and complexity of single-facility diversion that can be simulated within a model that integrates with the larger Cyclus ecosystem.

Other efforts have focused on coupling Cyclus to high-fidelity neutron transport codes for depletion modeling, such as OpenMC [15] and ORIGEN [84, 85]. These capabilities have not yet been used in nonproliferation applications but could be combined with the other medium-to-high fidelity models to study material unaccounted for (MUF) or other parameters that are sensitive to simulation fidelity.

Due to the high levels of effort required to replicate the facility-level complexity seen in special-purpose models such as PyRe and the challenge of creating similarly high-fidelity models across the fuel cycle, others have recognized the potential to generate notional safeguards in post-processing.

Burke *et. al* used simulated nuclear material movements as ground truth to generate data from sensor models that ranged from images to mechanical (vibrational) and temperature data [36]. However, once again the ability of that work is limited by the ability to simulate the nuclear material movements with enough spatial and temporal fidelity such that simulated sensor data can be of value.

2.3.2 Safeguards-focused process models

The Separations and Safeguards Performance Model (SSPM) tool, developed by Cipiti *et. al* has focused on developing high-fidelity process models for individual facility types of interest to the safeguards community [86]. Although the tool was not designed to model the entire life cycle of nuclear material, it has developed extensive process models, including relevant process and safeguards measurements for facilities of high safeguards interest, such as aqueous reprocessing [87] and pyroprocessing [88]. As SSPM and other process models develop more facilities across the nuclear fuel cycle while other lifecycle-focused simulations (such as the ones detailed in this dissertation) inch closer to process modeling, there is potential for future work to meet in the middle. Linking together a nuclear fuel cycle simulator such as Cyclus with a chemical process model such as SSPM could push the boundaries of realistic modeling for safeguards applications.

2.3.3 Sensitivity analysis and uncertainty propagation

Multiple prior efforts have focused on propagating measurement uncertainty in nuclear fuel cycle simulators, not all for primary purposes of nonproliferation and safeguards analysis [89, 90, 91]. Among the tools mentioned above, SSPM can conduct error propagation and calculation of MUF [92] on their models, and MUF analysis for pyroprocessing was demonstrated in PyRe [83].

Others, such as Shugart, built tools for uncertainty propagation, specifically for safeguards purposes [93]. Shugart's dissertation included MUF estimation based on data produced using the VISION simulator.

Another subfield of research increasingly integrating nuclear fuel cycle (NFC) simulations is nuclear archaeology, which aims to recreate documentation of nuclear-weapons-related activities from limited data. When trying to string together uncertainties not just from one facility but across the entire fuel cycle, several efforts have relied upon or integrated directly with NFC simulators to generate nuclear material inventories [94], including work by Bormann and Schalz to couple Cyclus to a Bayesian inference tool [95, 96]. Schalz recently built on this effort by using Cyclus to assess several possible fuel cycle strategies that Pakistan, a non-signatory State to the NPT with a declared nuclear weapons program, might have taken to obtain their fissile material stockpiles [29].

2.3.4 Modeling realistic facility behaviors on the appropriate timescale

The Cyclus models developed by McGarry [16] include facilities with behaviors designed for use in nonproliferation-focused simulations, such as randomized requests to divert highly enriched uranium [97] and a regional proliferation model [98]. These behaviors were integrated directly into archetypes within the mbmore packages and thus are not available to other and more commonly used archetypes, such as the ones in the Cycamore package.

McGarry's work indicates the value of more complicated sets of behaviors and transactions by facilities in safeguards-focused simulations and analysis. Existing behaviors, which assume that day-to-day fluctuations and the particulars of shipments between facilities are averaged out throughout a month-long time step (or longer), are not adequate in the context of safeguards simulations, where behaviors of interest may happen on the level of hours or days.

This dissertation includes several projects aligned with the same goal: to merge the motivation and methods of international safeguards with the tools and best practices of system-scale nuclear fuel cycle simulation.

Chapter 3 demonstrates how Cyclus, a flexible fuel cycle simulator, can be adapted to perform APA, which sets the foundation for this dissertation proposal by showing that system-scale nuclear fuel cycle simulators can be adapted to perform safeguards analyses.

Chapter 4 identifies key gaps in current Cyclus capabilities that limit the usefulness of simulations to safeguards analyses, namely a need to represent smaller units of space like material balance areas and patterns of movement on the timescale of days, and proposes additions that implement these capabilities. With these new capabilities, generating an entire State's worth of nuclear material movements becomes possible, which can be translated into synthetic nuclear material accounting reports.

Chapter 5 proposes a tool to generate nuclear material accounting reports from a Cyclus simulation, using the exact IAEA-created reporting style called Code 10.

Due to the sensitive nature of modeling entire States' worth of nuclear material, Chapter 6 proposes a systematic set of nuclear fuel cycle scenarios that capture a breadth of realistic reactor technologies and fuel cycle facilities that can be used to demonstrate a fuel cycle simulator's capabilities.

Finally, the new tools and behaviors will be demonstrated on several fuel cycle scenarios in Chapter 7, and Chapter 8 concludes.

3 ACQUISITION PATH ANALYSIS

Acquisition path analysis (APA) is a structured technique to assess nuclear fuel cycles objectively using a graph-based approach to nuclear material movements. The analysis should be reproducible and reduce the amount and subjectivity of expert judgments needed in international safeguards implementation. It was developed as part of this thesis and described as an aspect of the State-Level Concept (SLC), a holistic approach to safeguards customized to each State's fuel cycle and technical capabilities.

This work presents the first attempt to demonstrate that an agent-based nuclear fuel cycle simulator can be used as a platform to conduct APA. The chapter shows that a tool that was primarily used for long-term nuclear energy planning and evaluation can also be applied to the techniques of interest to international safeguards.

CYCLUS attempts to optimize transactions between agents in a dynamic resource exchange (DRE), designed to replicate a market-based system [99]. At every time step, active agents request commodities, and then agents have a chance to respond to requests if they can provide the desired commodity. This information is compiled into a single exchange graph, which is then solved using a minimum cost formulation to determine a feasible and optimal solution. The finalized exchange is a graph of supply-request pairs that represent material transactions between agents, which is executed at the end of the time step.

The purpose of the DRE is to determine an optimal set of commodity transactions between agents at a given timestep. Optimized transactions are valuable for the traditional use of dynamic nuclear fuel cycle simulators, which is to study technology transitions or resource-use optimizations, because only one solution to the supply and request portfolio is required for any timestep.

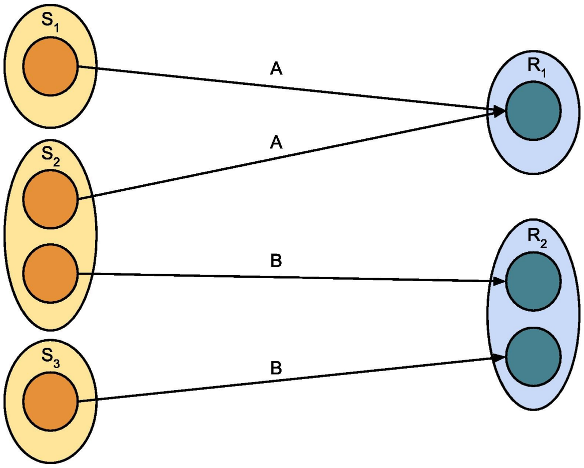

Figure 3.1: An example exchange graph [99]

3.1 Representing a Fuel Cycle as a Directed Graph

In the context of the SLC, however, every potential transaction of material between agents must be considered as a possible step in an acquisition path. For this reason, the TRAILMAP CYCLUS expansion module was developed to extend the consideration of commodity transactions to all possible requester-supplier configurations.

The model represents a nuclear fuel cycle as a finite directed graph, or digraph D, where individual agents u, v, w are nodes in a set V, and plausible commodity transactions are represented as edges (x, y) in a set E that have a source and a target node [100].

$$D = (V, E) \tag{3.1}$$

$$V(D) = \{u, v, w, \dots\} \tag{3.2}$$

$$E(D) = \{(x, y),\ (x, y) \in V^2\} \tag{3.3}$$

To capture more complicated plausible material movements, the model also allows for *multi-edges*, when two or more edges share the same source and target node. When multi-edges occur, the definition contains an additional incidence parameter, ϕ, to differentiate between two edges with the same source and tail node.

$$E = (x, y, \phi) \tag{3.4}$$

In the case of the nuclear fuel cycle, all graph edges are directed, and therefore multi-edges are more appropriately called multi-arcs. Consider the graph in Figure 3.2 with two nodes, $V(D) = \{v_1, v_2\}$ that represents an enrichment and a fuel fabrication facility. Multi-arcs $(v_1, v_2, 1)$ and $(v_1, v_2, 2)$ can be used to represent similar commodities that have a meaningful distinction, such as low enriched uranium (LEU) and highly enriched uranium (HEU). Multi-arcs can also cover different commodities, such as a reactor that can accept both uranium and mixed-actinide nuclear fuel.

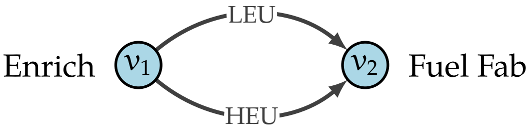

Figure 3.2: Enumerating simple paths can recognize multi-edges and create separate paths based on each multi-edge

Paths are graphs containing ordered sequences of steps between vertices. Because the graphs considered here are all digraphs, all paths have distinct source and target nodes, connected by zero (directly from source to target) or more inner vertices.

$$P = (V, E) \tag{3.5}$$

$$V(P) = \{(x, y, z)\} \tag{3.6}$$

$$E(P) = \{((x, y), (y, z))\} \tag{3.7}$$

A path P is said to be “in” graph D if $V(P) \subset V(D)$ and $E(P) \subset E(D)$. If a graph contains no multi-edges, P can be described uniquely by $V(P)$, otherwise $E(P)$ must be used.

Once paths have been enumerated, interactive analyses can be conducted to query and simplify the data before any Cyclus simulations are run. Following the precedent set by Cyclus, Trailmap was designed with a "plug-and-play" architecture that dynamically loads archetypes (software models of a facility or area) at run-time. This process loads the grammar that each archetype uses to interact with the simulation, such as commodities to request from or offer to the market. Trailmap takes advantage of these grammar definitions to analyze Cyclus input files directly, without having to make assumptions about any archetype.

Because the syntax of state variables for any archetype is not presupposed, new or closed-source archetypes (unknown to developers) can still be analyzed. Many potential users and archetype developers have sensitivity concerns, such as export controls and proprietary considerations that could limit their ability or desire to make their archetypes open source. The code base of Cyclus itself, along with some of the archetypes developed at several institutions, such the University of Illinois at Urbana-Champaign and University of Wisconsin–Madison, remain open source. Using this model of dynamically loading archetype grammar, APA can still be conducted using any archetypes written for Cyclus.

3.2 Acquisition Path Analysis

Conducting APA requires the ability to represent multiple types of diversion and their associated acquisition paths [101]. The four misuse path steps are shown in Figure 3.3. They may be combined to produce a full acquisition path that results in material suitable for use in a nuclear explosive device.

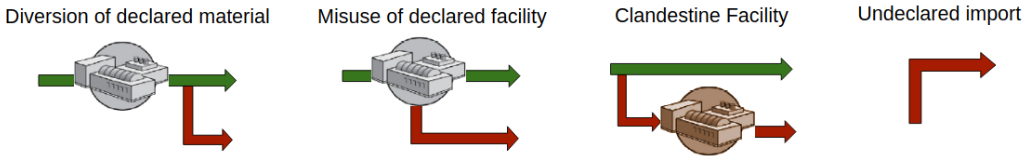

Figure 3.3: Four path steps to capture in acquisition path analysis

1. Diversion of declared material could happen from an MBA, or during the course of being transported between MBAs. Hypothetical examples include:
   - Uranium metal at a research facility goes missing.
   - A fresh fuel shipment from a fuel fabrication plant does not arrive at its destination;
   - A Cherenkov viewing device checks a used fuel assembly and finds that one fuel pin is not glowing. It has potentially been replaced with a dummy (non-fuel) element
2. Misuse of a declared facility could present as either operating a process when it is declared non-operational or producing nuclear material that is not declared. Hypothetical examples include:
   - An enrichment plant uses low-enriched material rather than natural uranium (NU) as feed to produce a higher enrichment than declared;
   - A reactor declares that it is shut down, but actually continues to operate
3. A clandestine facility is any facility or process that should be declared but is not. Hypothetical examples include:

  - A hot cell capable of reprocessing UNF is built and not declared;
  - A research institution declares owning no nuclear material or conducting no related research, but conducts research on laser isotope separation.

4. Nuclear material is imported from another State without declaration. Hypothetical examples of undeclared import include:

  - Undeclared import of depleted uranium targets from another State;
  - Undeclared import of enriched UF_6

TRAILMAP begins by using CYCLUS to identify all installed archetypes that exist on the user's machine. In this process, it identifies the key terms that will be present in the input file structure, in-commodities and out-commodities, a generalized term for any notion of material, an economic unit, or information that either enters or leaves a facility. Commodities are typically nuclear materials, but they could also represent money or critical components such as rotors.

Once TRAILMAP has identified the archetypes that exist on a user's machine, then information can be processed from a CYCLUS input file. TRAILMAP only supports the XML format of a CYCLUS input file.

3.2.1 State-Specific Information

As in any State-level safeguards analysis, the first step is compiling all relevant State-specific information, including declared facilities, processes, and import of material, but also potential undeclared facilities, processes, and import of material. Although this work is part of an effort to minimize the use of expert judgment and the potential for subjective reasoning in safeguards implementation, it is not yet possible to gather all necessary info to build a CYCLUS input file without subject matter experts. Information gathered and synthesized in this phase includes but is not limited to the following facilities and activities:

- Declared facilities
- LOFs
- Nuclear fuel cycle-related capabilities
- State system of accounting for and control of nuclear material (SSAC)
- Research and Development (R&D) activities
- Anomalies or inconsistencies identified in prior evaluations

Each of the above is important to the safeguards evaluation process [66, 101]. This is not a comprehensive set of State-specific factors used in the process of safeguards implementation, but rather the sub-set necessary for conducting APA. Beyond the scope of this research, the IAEA goes on to integrate the results of an APA with additional State-specific factors such as the type of safeguards agreement in force and prior safeguards conclusions (See Appendix B). This information can come from State accounting reports, declarations[1], electronic mailbox declarations [56, 102], and open source as well as other information provided by third parties [78].

One way that the dynamic capabilities of Cyclus can be advantageous is in considering processes deemed beyond the current technical capacity of a State, but are either being pursued under R&D or imported from another country. Within a dynamic fuel cycle simulation, this can be represented as a facility that does not get deployed in the simulation for a given amount of time based on the estimated time to develop that technical capacity.

3.2.2 Building a graph

Each facility in an input file is represented in the network as a node $v_i \in D$. For each facility's incoming commodities, all other nodes are searched to identify facilities

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[1] State accounting reports are the reports required of States that have concluded a CSA. Declarations are the additional information provided by States that have an AP, including States who have item-specific or voluntary offer agreements instead of a CSA

that can provide the desired commodity. When such a linkage is made, an edge (v_i, v_j) is added to the graph. The data structures that encode information about nodes and edges are intentionally flexible such that information such as the flow capacity of an edge or whether or not a particular facility is clandestine can be added.

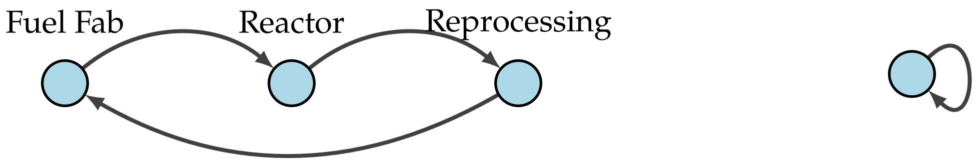
The creation of graph D is agnostic to the archetypes deployed and therefore does not hard-code any materials being traded or the edges they will flow through. In effect, this allows for the fidelity of a simulation to be raised or lowered by the user as needed and enables future facility models or unique commodity trading schemes without changes to the structure of TRAILMAP. A lower-fidelity simulation, for example, may use simplified archetypes such as SWU-based enrichment calculations (such as `Cycamore:Enrichment`), or a reactor that creates spent fuel based on recipes instead of any in-simulation depletion calculations (such as `Cycamore:Reactor`). The fidelity could be increased either by replacing archetypes with more realistic physical models and/or by increasing the set of facilities modeled by deploying MBAs throughout the fuel cycle.

Once a directed graph is built, conducting a modified depth-first search starting with each source node in the network will produce an enumeration of possible paths between the source and any target node [103]. A typical use case may designate mining facilities or import points as source nodes, but can also be set up to represent the import of material by adding a dummy node to indicate an unknown origin, or by adding additional facilities representing the true source of the material. This enumeration does not quite reach the designation of acquisition paths yet, because most fuel cycles will contain paths that do not end up producing weapons-usable material.

Users are encouraged to create a dummy sink facility in their input file whose sole purpose is to request weapons-usable material, typically defined as plutonium or HEU. Then the original list of all paths can be sorted for the weapons-usable material collector to produce the desired list of acquisition paths. See Section 3.3 on the metrics that can be produced.

3.2.3 Cycles

A traditional path cannot contain repeated edges. However, nuclear material flows can return back to a previous node, most commonly when UNF is reprocessed, and some of the material is recycled back into nuclear fuel, so additional handling is required to represent these systems. Figure 3.4 shows the two ways that path steps can repeat. A cycle must include at least two nodes, and begin and end with the same node. A loop is where an edge begins and ends with the same single node. The depth-first search algorithm, as deployed using *networkx* [104] in TRAILMAP, has no functionality to account for cycles or loops. Loops are defined as cycles that leave and return directly to the same node[2].



(*a*) *A cycle includes at least two nodes*

(*b*) *A loop is an edge that leaves and returns to the same node*

Figure 3.4: Types of repeating path steps

One simple path through the system as shown in Figure 3.5 would be [Enrichment, Fuel Fab, Reactor, Reprocessing, Waste], however, a cycle of (Fuel Fab, Reactor, Reprocessing, Fuel Fab)[3] presents a challenge to represent. A path could be drawn

---

[2] Some conventions include a two-node cycle as a loop, while others do not. For the purposes of this work, a loop only refers to an edge with the same source and target.

[3] Which could also be represented as (Reactor, Reprocessing, Fuel Fab, Reactor), and (Reprocessing, Fuel Fab, Reactor, Reprocessing)

from [Enrichment, Fuel Fab, Reactor, Reprocessing, Fuel Fab], but this is not useful because the Fuel Fabrication plant is unlikely to be the conclusion of nuclear material movement.

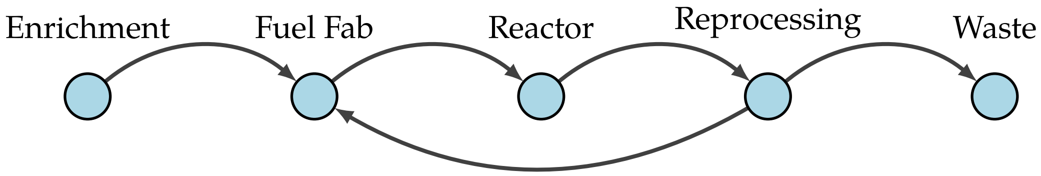


Figure 3.5: Some fuel cycles actually have cycles

The most straightforward uranium and plutonium paths do not require closed fuel cycles. However, there may be instances where material could be diverted after it has been reprocessed and reintroduced into an earlier point in the fuel cycle.

Simple cycles can be returned alone, for example as (A, B, C, A), (B, C, A, B), or (C, A, B, C) from Figure 3.6 assuming that the rest of the fuel cycle is comprised of simple paths. Given that a cycle has no beginning or end, it is equally likely to be reported with any of the nodes in the first position. For example, Figure 3.7 contains equivalent graphs (a) and (b), even if one layout is interpreted as more physically meaningful.

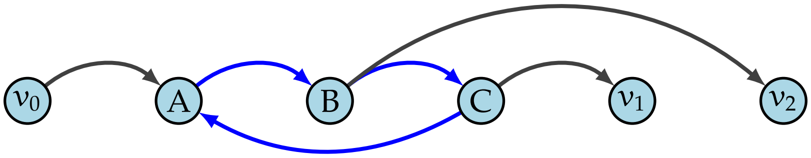


Figure 3.6: TRAILMAP *can return simple cycles*

When requested, TRAILMAP will seek to combine the simple paths and simple cycles in a logical manner. All nodes in a given simple path will be checked for presence in any cycles. If so, the cycle will be "rolled" such that the first position in the cycle is the leader, or first vertex that is present in both the cycle and the path.

(*a*) (*b*)

Figure 3.7: These cycles are identical and equivalent to (A, B, C, A).

For example, the cycle in Figure 3.6 could present in multiple ways, such as Figure 3.7(a) and (b). If the cycle is first identified as the version in 3.7(a), (C, A, B, C), it should be rotated so that A is at the beginning of the cycle, or (A, B, C, A) (3.7(b)).

Consider a graph, similar to the one in Figure 3.6, with the following simple paths: (v_0, A, B, C, v_1), (v_0, A, B, v_1), and rolled simple cycle (A, B, C, A). Since the cycle overlaps with both simple paths, each gets a copy with the cycle inserted where A was, and the full set of paths including cycles becomes

- (v_0, A, B, C, v_1)
- (v_0, A, B, v_1)
- $(v_0, (A, B, C), B, C, v_1)$
- $(v_0, (A, B, C), B, v_2)$

Limitation - Complex Cycles

This work only considers simple cycles, where only the beginning and end are repeated. The example cycles shown above, including the ones in Figure 3.7, are simple. A cycle embedded in another cycle, such as (b, c, d, f, g, h, g, i, b) from Figure 3.8, would not be simple since the node *g* is repeated. However, the cycle that does not touch node *h*, or (b, c, d, f, g, i, b), is simple and can be recognized in the paths from *a* to *e*.

When multiple cycles share nodes, they will be simplified into simple cycles if possible, but are not currently handled as a complex cycle. In the case of the two cycles in Figure 3.9, two simple cycles are present: (b, c, d, f, g, i, b) and (c, d, f, g, c). Each of these cycles can be identified and recognized as part of a potential path from

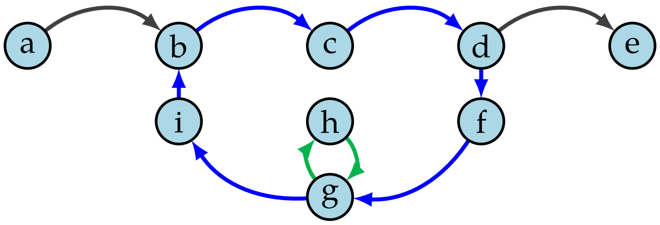


Figure 3.8: Complex cycle fully contained within another cycle

a to *e*. However, a complex cycle that intertwines the two, $(b, c, d, f, g, c, d, f, g, i, b)$ repeats several nodes and isn't currently handled.

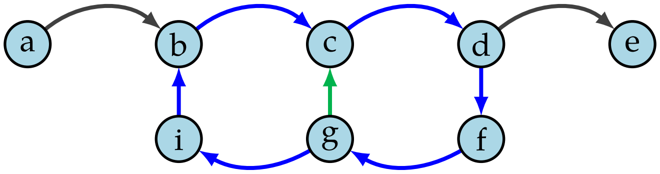


Figure 3.9: Complex cycle partially contained within another cycle

3.2.3.1 Multi-edges with cycles

Obtaining simple paths of a graph already considers multi-edges independently. For example, a graph as shown in Figure 3.10 would result in paths of [a, b, c, d] and [a, b, c, d]. Or, by edges lists with (u, v, k) where u is the head, v is the tail, and k is an edge index, $[(a, b, 0),(b, c, 0),(c, d, 0)]$ and $[(a, b, 0),(b, c, 1),(c, d, 0)]$, which more clearly reveals where the multi-edge is causing multiple simple paths arising from the same list of nodes.

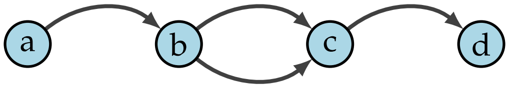


Figure 3.10: Enumerating simple paths can recognize multiedges and create separate paths based on each multiedge

However, the *networkx* function used to identify simple cycles does not recognize multiedges.

3.3 Metrics and Output

After building an acquisition path network, Trailmap can provide several useful filtering and sorting tools based on common lines of inquiry.

Producing a list of acquisition paths is only the first step in analyzing the set of fuel cycle facilities in accordance with the SLC. It does, however, produce the first point of information, the number of potential acquisition paths that must be safeguarded or discarded as either nonphysical or beyond the technical capabilities of a State. For example, one path that could be generated depending on how an input file is structured includes tailings material depleted in ^{235}U going to the mixed oxide (MOX) fuel fabricator before ending up at the dummy HEU/Pu collector facility. This path is based on the fact that the fuel fabricator would normally combine reprocessed plutonium with uranium to produce MOX fuel, so depleted uranium (DU) is on its list of potential incoming commodities. However, it is nonphysical for DU to enter a non-enrichment facility and exit as weapons-usable material, so this path can be discarded.

3.3.1 Based on Path Length

The simplest analysis tools are based on the number of steps in a given acquisition path. As with the other sorting and filtering tools, they can be used together, such as finding all paths with fewer than n steps, then sorting the result by shortest to longest.

1. **Sort Paths By Length**. Given the full list of paths, or a subset from another sorting or filtering option, they can be sorted from shortest to longest or vice versa.

2. **Shortest Path**(s). Identifies the path or paths that require the smallest number of path steps to reach weapons-usable material. In the example case, the shortest paths are misuse of the declared enrichment plant to produce HEU or diversion of UF_6 to the undeclared enrichment facility.

3. **Path Shorter than** n

4. **Longest Path**(s), . Identifies the path or paths that require the longest number of path steps to reach weapons-usable material.

5. **Path Longer than** n. All paths

3.3.2 Based on Presence or Absence of Particular Facilities

Users may want to identify paths that flow through a particular facility or type of facility of interest. Considering the wide range of queries that could arise, there are several ways of sorting by facility. A user can identify paths that include a specific facility, as well as specify locations along the path where that facility must occur. For example, a user may be interested in paths that begin from a particular Source node, or they may just want facilities with enrichment plants regardless of where the enrichment facility shows up. This notion is also extended to lists of facilities. Users can search for paths that contain either any or all of the facilities in a given set of facilities. Paths with a particular source and target node can be identified, and further simplified into node disjoint paths (see below). The path identified earlier as nonphysical could be sorted out using a search that identified paths including tailings facilities and the MOX fuel fabricator and discarding them.

3.3.2.1 Paths that include some, all, or none of a list of facilities

Several filtering options are available based on a single or set of facilities of importance. Paths can be identified based on the inclusion of all facilities of interest. When applied to more than one facility, this is an AND operation.

Paths can also be identified that must include one of a list of facilities, which may also be called one-or-more. For a single facility, this behaves identically to the previous metric. When applied to more than one facility, this is an OR operation.

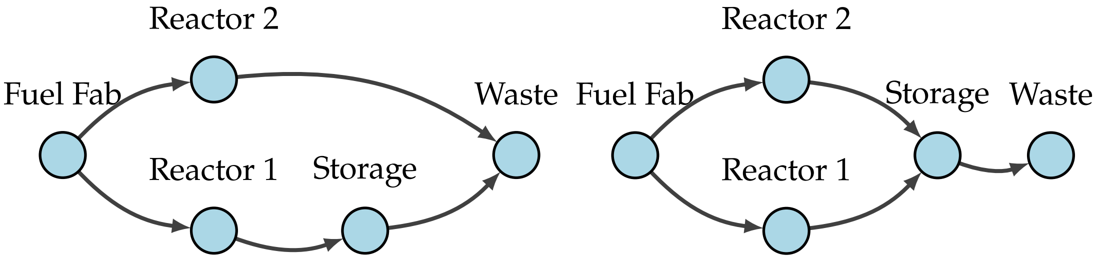
A related metric is paths that must include only one facility out of a set of options $(u, v, w, \cdots)$. This metric is only relevant for two or more facilities, otherwise it is equivalent to all paths with a given facility. This represents an exclusive-or (XOR) operation. This may be used when several facilities are present in an analysis and they may be considered interchangeably.

For example, an analysis may consider the potential for multiple types of uranium enrichment, such as gaseous diffusion and gas centrifuge. An analysis looking for paths that include enrichment could use both the regular OR operation and an XOR operation. Paths that include at least one enrichment or the other may result in paths that lead from one enrichment facility to the other, such as gaseous diffusion production of LEU from NU, and then to a gas-centrifuge enrichment plant (GCEP) for further enrichment from LEU to HEU. However, this path of double-enrichment could reasonably be captured by simplifying to only one enrichment plant producing HEU from NU, and the XOR metric would only return paths that step through one facility or the other.

Finally, paths that include none of the given facilities can be filtered from the total options. This returns paths that don't contain any of the given facilities in any position, including the source or target (beginning and end) nodes.

3.3.2.2 Node disjoint paths

Node disjoint paths are paths that have the same source and target node but share exactly zero other nodes (and correspondingly, edges). The graph shown in Figure 3.11(a) has node disjoint paths between the fuel fabrication and waste facilities, [Fuel Fab, Reactor 1, Waste] and [Fuel Fab, Reactor 2, Interim Storage, Waste], while Figure 3.11(b) has none because both paths share the storage node. However, in Figure 3.11(b) there are two node disjoint paths from fuel fabrication to storage, [Fuel Fab, Reactor 1, Storage], and [Fuel Fab, Reactor 2, Storage].



(a) Two node disjoint paths from Fuel Fab to Waste *(b) Zero node disjoint paths from Fuel Fab to Waste*

Figure 3.11: Node disjoint paths

3.3.2.3 Cut-vertex

Given a set of paths from distinct vertices u to z, a cut-vertex(ies) w is a vertex that is present in every path. Cut-vertex analysis will be most useful on a set of paths that have already been winnowed down from an entire fuel cycle.

In example Figure 3.12, only d is a cut vertex between a and g. All of the following paths contain node d

- a, b, d, e, g
- a, b, d, f, g
- a, c, d, e, g
- a, c, d, f, g

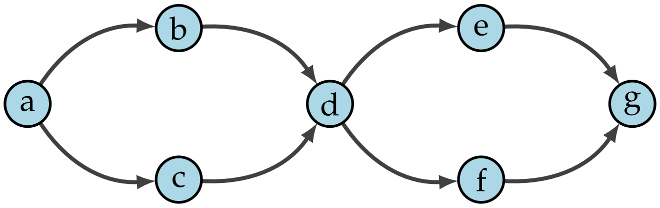


Figure 3.12: Node d is a cut vertex

3.4 Demonstration

The functionality of Trailmap is demonstrated using a simple model of a hypothetical State with a parallel civilian and military fuel cycle as shown in Figure 3.13. Both tracks share a mine, mill, and conversion plant. The civilian fuel cycle includes an enrichment plant with a tailings pile, a uranium oxide and a mixed oxide fuel fabrication facility, a light water reactor, a reprocessing plant, and storage facilities for used fuel and enrichment tails. The military fuel cycle includes a uranium enrichment facility with a tailings pile. For simplicity, only one facility of each type is defined in the simulation.

Using a fuel cycle simulator to conduct APA brings reproducibility and consistency, but the process still requires information, including expert judgement, to develop a Cyclus input file that captures the depth and breath of a State's past, present, and planned nuclear fuel cycle related capabilities. The following set of key information was defined by the IAEA as integral to conducting APA [101] and must be given as an input to Trailmap by developing a thorough Cyclus input file.

- Declared facilities and LOFs
- Declared flows of nuclear material
- Declared sites (if an AP is in force)
- Exports and imports of nuclear material
- Nuclear fuel cycle related research and development activities, signaling technologically feasible facilities and flows
- Uranium mines and concentration plants

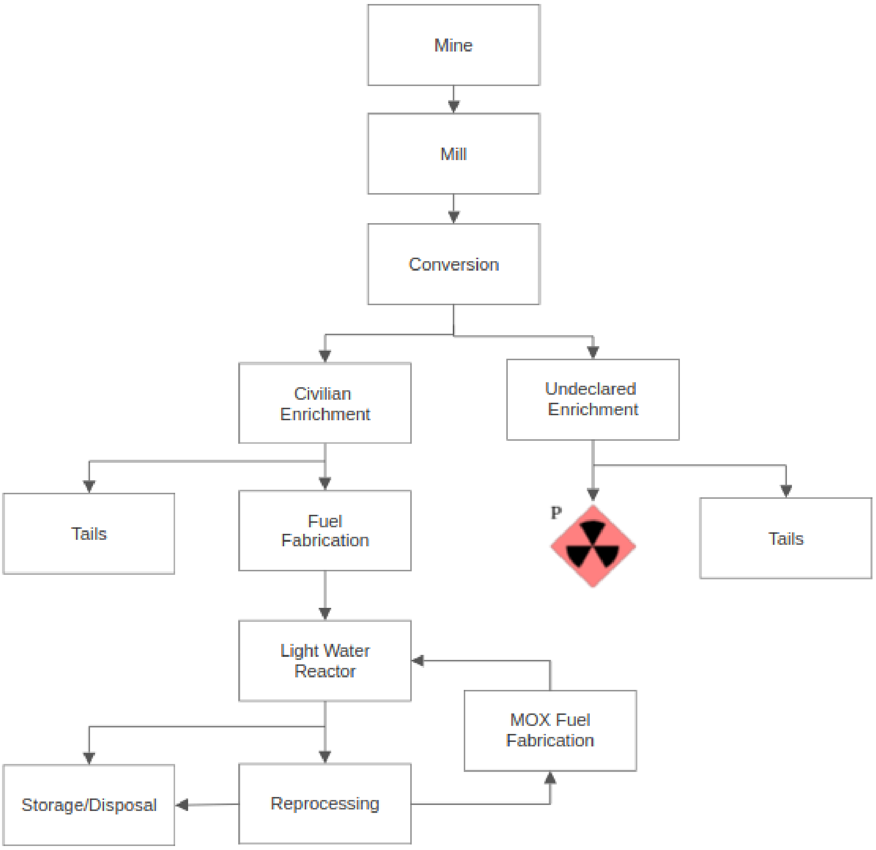


Figure 3.13: Example state for acquisition path analysis

- Holdings of source material which has not reached the composition and purity suitable for fuel fabrication or being isotopically enriched

TRAILMAP can enumerate and sort paths based on common criteria such as length of path, logical operations of a facility or list of facilities, and cycles. Like any APA, TRAILMAP is constrained by the information it is given. It is essential that State-specific factors like fuel cycle and fuel cycle related facilities and capabilities are adequately built into an input file such that all potential paths can be identified.

3.4.1 Visualizations

Paths, groups of paths, and even individual paths can be visualized using an interactive notebook. In Figure 3.14, the example fuel cycle is visualized disregarding some of the paths through tailings facilities.

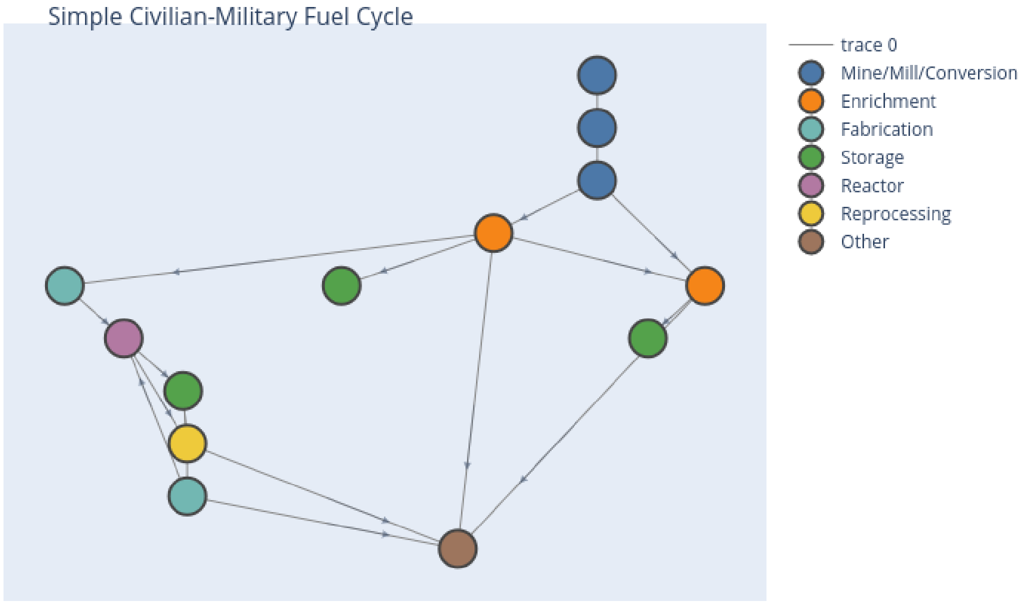


Figure 3.14: Visualized demonstration fuel cycle

Hovering over a node highlights the name of the node as defined in the input file (Figure 3.15(a) and highlighting an edge shows the commodity flowing as well as the source and target node (Figure 3.15(b)). Future feature development should include more detail such as edge capacity in the visualization.

Individual acquisition paths can be overlaid on the network as shown in Figure 3.16.

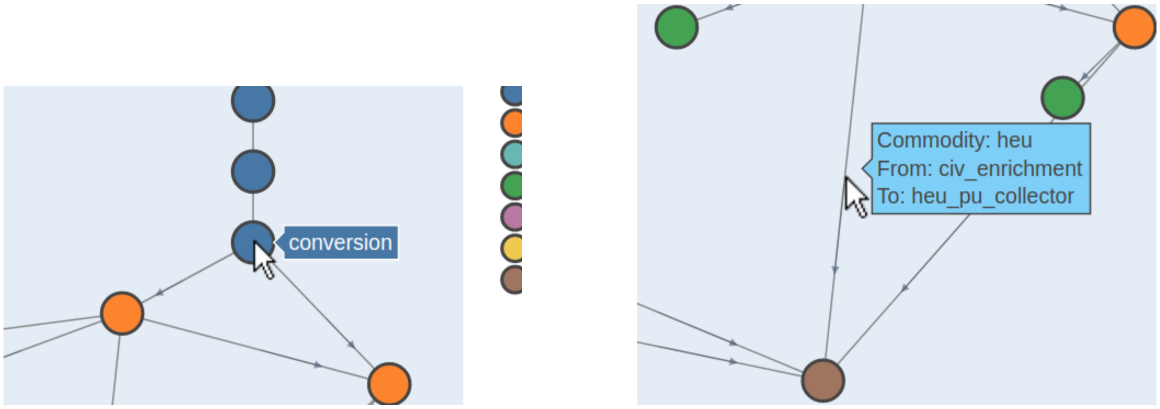


Figure 3.15: *Hovering over features of the graph*

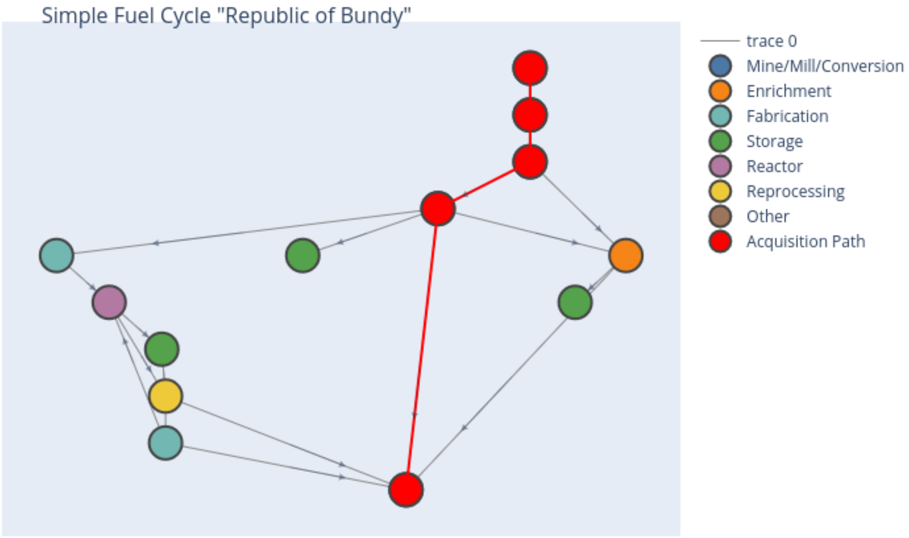


Figure 3.16: *Acquisition path overlaid onto a graph*

3.4.2 Conclusion

Conducting simple APA with Cyclus was the first step in demonstrating how cradle-to-grave nuclear fuel cycle simulation can be useful to international safeguards challenges. The development of Trailmap was an important foray into merging the tools of NFC simulators with the methods being developed for State-level approaches in international safeguards. However, this work was limited by the publicly available information on the metrics and technical objectives of APA that are of interest to the IAEA.

The following chapters more effectively address current opportunities to improve safeguards modeling and analysis using nuclear fuel cycle simulation tools.

The limiting factor of conducting APA in a nuclear fuel cycle simulator is not the graph theory or code implementation but rather the fidelity of spatial units and the need to integrate more detailed State-specific factors. The other sections in this chapter address these issues more closely, and together, this prepares the groundwork for additional development and demonstration of APA in fuel cycle simulators in the future.

4 AGENT INVENTORY MANAGEMENT AND PACKAGING

Over the past decade, several efforts have been made to advance the capability of nuclear fuel cycle simulators to conduct international safeguards-relevant analyses. In many cases, this has involved decreasing the length of time represented by a single time step. One time step per month may be enough temporal fidelity for long-term nuclear energy planning studies, but this is not adequate for safeguards. For example, realistic State accounting reports that use the IAEA-developed Code 10 data format must be able to report the day in which nuclear material was moved, not just the month. A hurdle to these efforts is the simplicity of agent behaviors that are implemented across the core Cyclus facilities, called Cycamore, and their inability to replicate realistic NFC behaviors on the order of day-long time steps.

There are three core processes that are executed at each time step in an ABM nuclear fuel cycle simulator. The first process governs how nuclear materials and other commodities of interest are handled, refined, or otherwise modified within an agent. Each agent is responsible for handling the nuclear materials it owns. This work comprises the bulk of the physics and chemistry-based modeling of a fuel cycle simulation, as agents are typically designed to represent a physical process in the nuclear fuel cycle.

The other two processes are how agents determine when and how much feed (product) to request (offer) the other agents in the simulation, and how the framework solves the network of requests and offers. In Cyclus, the optimal exchange of resources is determined by the dynamic resource exchange (DRE), which was primarily developed by Gidden as a graduate student at UW–Madison [99].

The handling of requests and offers to the DRE by agents has historically been the least developed of the three processes. Because this aspect of Cyclus has not been continually advanced along with development of agent behaviors and the DRE, the lack of flexibility and unrealistic patterns of material movement are the current limiting factor in increasing simulation fidelity. This work aims to enable agents in the Cyclus ecosystem to incorporate more complex and realistic requesting and offering behavior.

Instead of identifying a single step in the nuclear fuel cycle and increasing agent fidelity, this work enacts a more generic set of behaviors that will be useful across the NFC. Implementing these behaviors in the Cyclus toolkit makes these behaviors available to any archetypes implementing the toolkit. This applies to the entire Cycamore suite of archetypes, but in keeping with the plug-and-play ethos, this could also aid third-party archetype developers wishing to implement similar behaviors.

The ability to model more complex behavior on both sides of the DRE, requesting and selling commodities, has been added to the Cyclus kernel and in several demonstration archetypes. Each one arises from a careful reflection of system behavior seen in the NFC and that could not have been easily implemented simulation-wide with pre-existing tools. The terms requesting and offering are used interchangeably with buying and selling behavior, although this work does not include economic modeling or the financial aspects involved in nuclear materials moving throughout the nuclear fuel cycle.

First, in Section 4.1 I describe the process for moving from a facility-based deployment of agents to an MBA-based deployment, where multiple agents collectively represent a single facility. A system-wide random number generator is introduced in Section 4.2 to support the increased use of stochasticity in modeling. Periodic, random, and continuous review inventory policies are introduced in Sections 4.3, 4.4, and 4.5. A new system for packaging resources and implementation into the selling side of the DRE is discussed in Section 4.6.

4.1 Building a simulation for international safeguards analysis

To meet the fidelity needed for safeguards modeling, movements between MBAs within a facility must be simulated and recorded as transfers of nuclear material.

Deploying parts of a nuclear fuel cycle for an energy system is typically focused on simulating nuclear materials at the facility level. Especially when a month-long time step is used in a simulation, there is no need to explicitly model when a certain material is in a storage location versus in-process.

When simulating nuclear material movements and processes for international safeguards, the relevant spatial fidelity is the MBA and KMP. Movements between MBAs within the same facility trigger an inventory change in the same way that a receipt of material from another facility would. Facilities with multiple MBAs must then have at minimum the same number of agents as MBAs, because Cyclus tracks material movements between agents, not within. In practice, simulations are better served by separating all storage locations from processing agents so that even single-MBA facilities are represented by multiple connecting agents. Figure 4.1 shows an example of a fuel fabrication facility split into five agents.

MBA1 and MBA3 are comprised of a single agent each, while MBA2 includes three agents. Movements of nuclear materials from the pellet fabrication process to rod loading agents are recorded in a Cyclus simulation but would not trigger an inventory change to be reported to the IAEA.

Splitting facilities into many agents introduces some additional complexity into

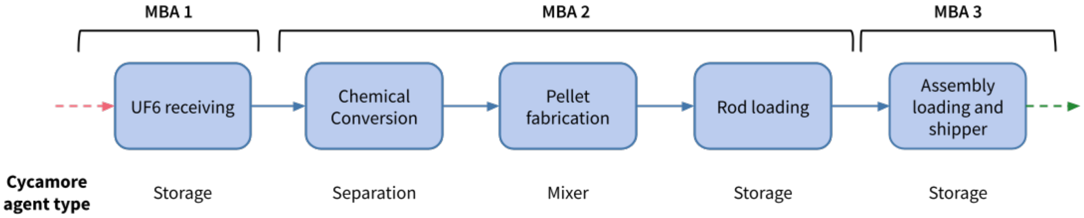


Figure 4.1: A single facility, here a fuel fabrication plant, may be represented with several agents in a simulation. At least one agent must be present per MBA, such as MBAs 1 and 3. Multiple agents may also represent a single MBA, especially when chemical processing of bulk material occurs in that MBA.

simulation development, as Cyclus does not natively support individual agents restricting their trades to specific agents. Restriction of trading can be done with regions or institutions [23], but is not well suited for modification to restrict trading partners for individual agents.

Instead, users must create unique facility-specific commodities when deploying multiple identical facilities to ensure the intended flow of materials. Figure 4.2 shows how unique commodities must be used for the flow of fuel from the fresh fuel vault to the reactor to the separate UNF pool.

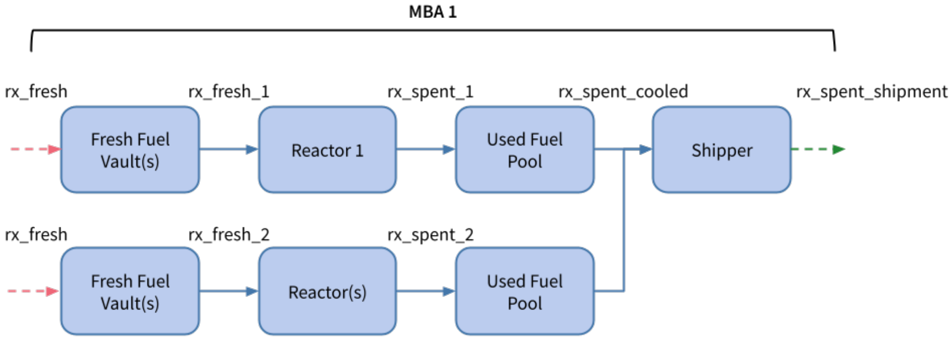


Figure 4.2: Unique intra-facility commodity names must be used to ensure repeated agents don't send nuclear materials to the wrong downstream agent or even the wrong facility.

This strategy is used in Chapters 6 and 7 to ensure nuclear material flows are simulated at the MBA level for international safeguards, but it can result in much longer runtimes as the DRE must partition many more graphs for all of the unique facility-specific commodities.

4.2 Random number generator

The addition of a pseudo-random number generator (PRNG) into Cyclus supports wider use of stochastic behaviors across a fuel cycle simulation.

A few archetypes have historically incorporated randomness into their behavior, including the `mbmore` archetypes `RandomEnrich` and `RandomSink` [16]. Historical implementations have placed the burden of random number generator management on individual agents. If expanded across multiple agents in a simulation, a simulation could end up with many different PRNGs, each with its own seed and potentially using different algorithms for number generation. This scenario would likely result in less-than-ideal practices such as seeding all agent PRNGs identically, resulting in identical sequences of numbers used for each agent. Instead, random number generation has been moved to the Cyclus simulation kernel.

A single PRNG, a Mersenne twister 19937 generator from Boost [105, 106], is managed by the Cyclus kernel for every simulation. The Mersenne twister [107] is a widely used generator due to its long cycle length of $2^{19937} - 1$ steps and relative speed. Users may set a seed; otherwise, a standard fixed value is used so simulations are repeatable by default.

The distributions available for agents to access are shown in Table 4.1. Two processes have been developed for agents to access a random number at any point throughout the simulation. If agents rarely need to generate a random number or will be generating random numbers with parameters that change frequently, agents can call the simulation context and request a single number from a specified distribution. For example, to access one `double` drawn from a truncated Gaussian:

```
double random_number_trunc_normal =
    manager()->context()->random_normal_real(mean, standard deviation,
                                             min, max)
```

Table 4.1: Random distributions available through the CYCLUS kernel

Distribution	Double	Int	Parameters
Random	✓	✓	
Zero to one	✓		
Uniform	✓	✓	Min, max
Normal	✓	✓	Mean, standard deviation. Optional: min, max
Binomial	✓	✓	Trials, probability of success
Negative binomial	✓	✓	Successes, probability of success
Poisson	✓	✓	Mean
Exponential	✓	✓	Lambda
Binary	✓	✓	Probability of success, value if success, value if failure

Many agents will frequently generate numbers from a single distribution. In this case, agents can create a member variable and manage the distribution, which will still pull from the single kernel-managed PRNG. For example, an agent can create a uniform `int` distribution between a fixed minimum and maximum value:

```
cyclus::IntDistribution dist = cyclus::UniformIntDist(
    new cyclus::UniformIntDist(min, max));
```

Obtaining a random number from the distribution can be done easily by sampling:

```
    int random_number = dist.sample()
```

4.3 Periodic inventory strategies

A set of inventory strategies were developed based on cycles of active and dormant behavior, collectively called period inventory strategies, to support more complex material buying behavior.

Cycamore is a set of facility models, called archetypes, developed for the Cyclus ecosystem. Many Cyclus users develop and incorporate their own third-party archetypes into simulations, but the Cycamore models are used in almost every Cyclus simulation because they present all the functionality needed to develop a complete if simple fuel cycle.

However, nearly all of the Cycamore archetypes were designed to try to keep their inventories as full as possible over time. Whenever space is available, such as when their product is traded to another agent, they immediately attempt to buy more feed, in order to produce more product(s). The space made available by the processing of feed results in a request for that amount of feed to return the inventory to maximum capacity.

Consider a simulation agent i at time step t_n requesting a single commodity. The agent has a maximum allowable inventory of L_i for the requested commodity, and holds existing inventory from the previous time step, $I_i(t_{n-1})$. For the Cycamore agents, this results in a request $b_{r,i}$ at any time step corresponding to the space available,

$$b_{r,i}(t_n) = L_i - I_i(t_{n-1}) \tag{4.1}$$

Here the request $b_{r,i}$ is simplified as the request quantity for clarity, but the request is actually comprised of a quantity and a constraint coefficient conversion function that incorporates additional constraining information such as material quality. Gidden and Wilson [99] define the full formulation of the Nuclear Fuel Cycle Transportation Problem used in the DRE, but for our purposes, $b_{r,i}$ can be considered as a desired mass of a specific commodity.

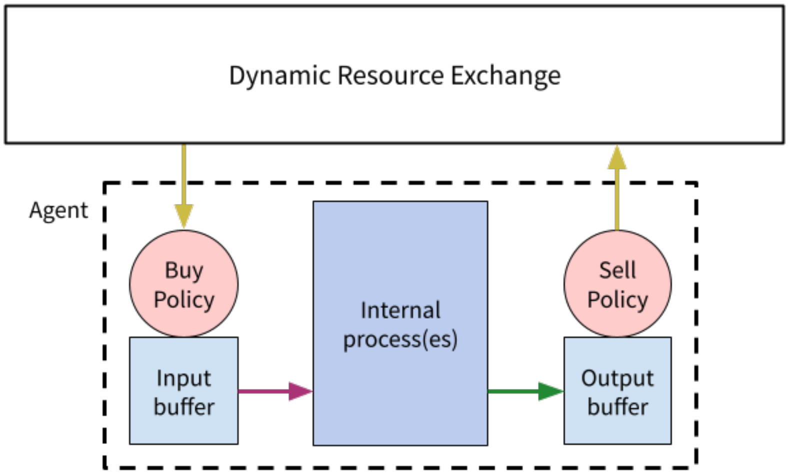
This assumption is not adequate for simulations with time steps that are one day long, rather than one month like is common for fuel cycle transition modeling. This presents a challenge to increasing the temporal fidelity of CYCLUS simulations. There is no system-wide mechanism to restrain all agents' behavior when "maintain full inventories at all times" is no longer a reasonable material management strategy.

One solution to fix this issue would be to change the internal behavior of every CYCLUS agent. The internal behavior of every known open-source CYCLUS agent could be modified to support new inventory drivers. But a more effective way to throttle the movement of material into an agent is by adding capabilities that affect the interface between agents and the simulation kernel, allowing new developments to be generic enough that multiple agents can reuse them without significant overhead. These strategies have been added to the CYCLUS toolkit, specifically the Material Buy Policy, allowing any agents to use these inventory management tools.

The Material Buy Policy and Material Sell Policy are tools that an archetype developer can integrate into their facility models to manage the buying (selling) of materials to the DRE. Shown in Figure 4.3, the policies tag onto either end of an archetype and manage the buying (selling) of the feed (product) material and manage the inventory of the input (output). When using them, an archetype developer can focus on developing the internal block, labeled "inventory" in Figure 4.3, pulling from the input inventory and pushing to the output inventory as needed.

The inventory management strategies here and in Section 4.4 are implemented

Figure 4.3: Material Buy and Sell Policies act as an interface to the DRE for an archetype, allowing archetype developers to focus on developing their archetype's internal processes.



into the Buy Policy, and packaging, detailed in Section 4.6, is implemented into the Sell Policy.

Binary behavior states are introduced into the Buy Policy to support additional control over an agent's demand for feed material, with several strategies to cycle between them. First, the active state preserves existing buying behavior. The new second state is dormancy. During a dormant state, agents will place no demands for their feed material, or incoming commodity, regardless of the space available. The default implementation of active and dormant cycling is a permanent active state. This is backward-compatible with previous versions of the software.

4.3.1 Fixed cycles

The most straightforward application of active and dormant cycles of behavior is characterized by two fixed values. Given a user-defined active length of time steps and dormant length of time steps, the agent regularly cycles between them. The active state allows regular behavior to proceed; if an agent does not have space in its inventory for new material, it will not place a request even during the active cycle. During the dormant phase, the agent may still process material already in its inventory, but will place no new requests for feed material regardless of space in inventory.

There are several ways this behavior can be used to model realistic patterns of material movement. One example is the work week. A facility may be on for five days and then off for two, as shown in Figure 4.4. Given a fixed demand for material per time step, a facility with fixed cycles processes less material than an always-on facility.

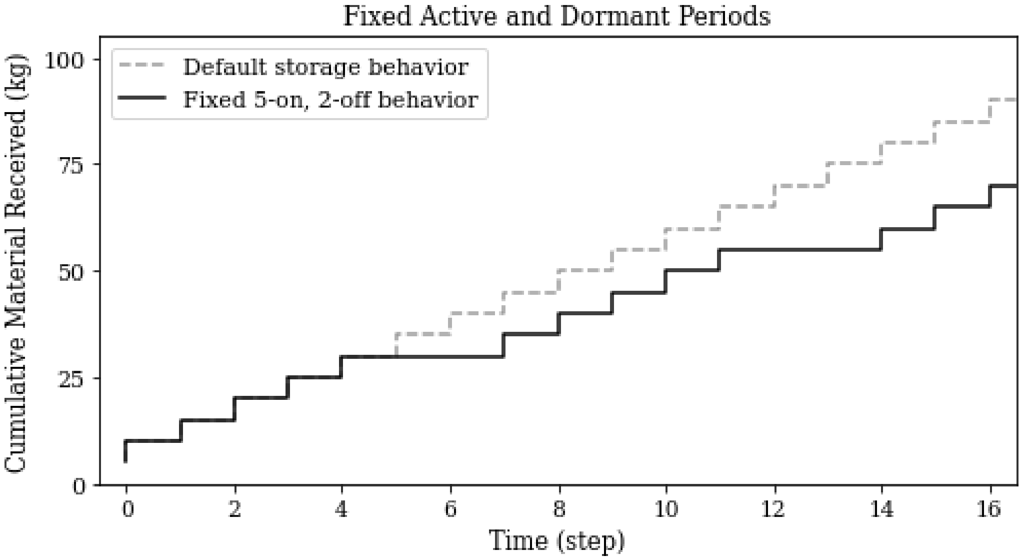


Figure 4.4: Active and dormant demand cycling with weekday on and weekend off behavior implemented in the Cycamore *storage archetype*

Another use of fixed cycling is for a process that implements production cycles, such as a facility shutting down on a regular cycle for planned cleaning, refurbishment, or other planned maintenance.

4.3.2 Random cycles

Stochasticity can be added to active and dormant cycles to replicate behavior that is periodic and (pseudo-)random. Users can generate random numbers through the Cyclus kernel-managed PRNG (Section 4.2) paired with a distribution of interest. Uniform and normal distributions are implemented in the kernel, but other distributions may be paired with the generator.

Adding random distributions to periodic review behavior allows more realistic buying patterns to be modeled. For example, a reactor facility would like its batch of fresh fuel to arrive a certain number of weeks before the outage so the assemblies can be unpacked, moved to the fresh fuel vault, and inspected. In reality, the dormant type between fresh fuel shipments will include a shipping window or tolerance, and therefore, the dormant length should not be a fixed integer.

Another use case of random cycles is to study the impacts of a "diverter" agent. A random buying request will make diversions less regular and more challenging to detect.

4.4 Randomness in size of request

The size of a feed material request can be restricted using random distributions. The distribution must have a maximum value no larger than the largest possible request, given the agent's restrictions on throughput, inventory space, or other mass limitations.

Applying a distribution to the request size can be combined with either periodic (Section 4.3) or continuous review (Section 4.5), such as shown in Figure 4.5.

Implementing stochastic behavior in request mass is useful in simulating the movement of bulk materials, where small variations in mass between containers are

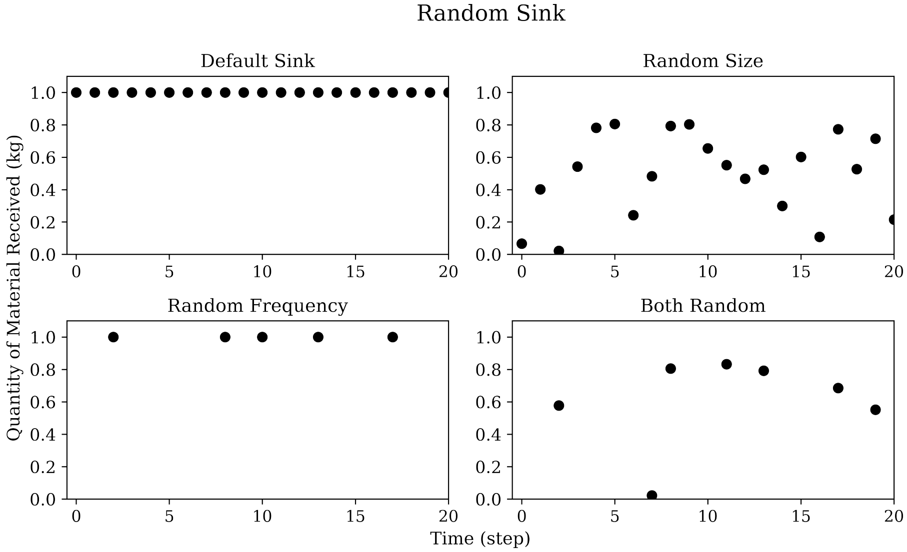


Figure 4.5: Use of active/dormant cycles and randomly-sized requests can be combined. Example using C*ycamore sink facility.*

expected. For example, a normal distribution could be used to sample masses for filling 55-gallon drums with uranium ore concentrate (UOC). Truncation values could be set at the minimum reasonable fill and the maximum regulatory fill limit.

Random behavior can be used to prevent multiple facilities from moving in lock-step, or to compare across simulations by varying the seed of the PRNG. Figure 4.6 shows the receipt of a `Cycamore:Sink` agent across simulations with different seeds. All agents sample their request size from a normal distribution $N(0.5, 0.2, 0, \infty)$ and request frequency from a uniform distribution $U(5, 15)$).This process can be used to bound a range of expected outcomes across a fuel cycle.

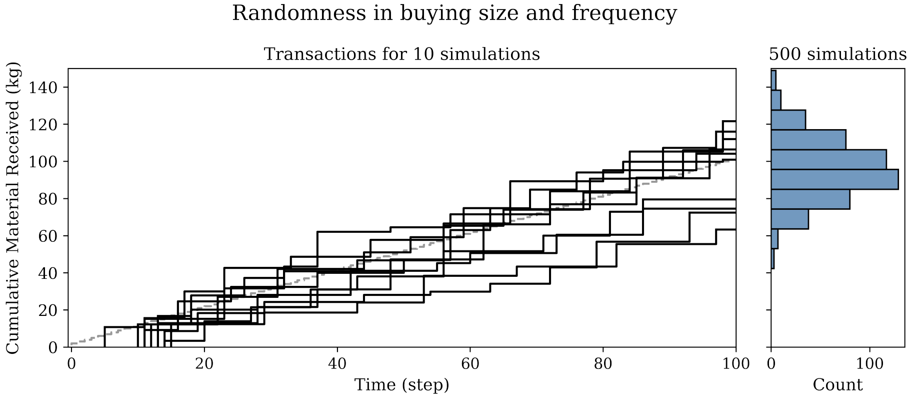


Figure 4.6: A range of expected values can be generated by running the same simulation with different seeds. Here, the randomness is sampled from normally distributed request size and frequency from a uniform integer distribution.

4.5 Continuous review inventory policies

One new capability to control the flow of nuclear material movements into an agent are continuous-review inventory policies. The previous default agent behavior is a type of continuous-review policy. Inventory is reviewed at each time step to determine the remaining inventory space.

The new policies described here introduce set points that govern when agents should attempt to restock their inventories, and in what quantities. Inventories are reviewed against these set points at each time step, but when the current inventory is outside these set points the agent remains dormant and places no new requests for feed.

Continuous-review policies are similar to the active and dormant cycles except they are driven by the quantities of material received by the facility rather than sampled from distributions.

4.5.1 Minimum/maximum inventory - (s,S)

In a minimum/maximum inventory policy, a facility will actively demand more material if it has an inventory below the minimum value, s, including when starting from zero. The agent places a request up to the maximum value, S as shown in Equation 4.2. Then the agent enters a dormant phase until the feed material has been processed and sold so that the facility inventory drops below s again. The requests for feed material are scaled at each time step t_n to fill the inventory back up to the maximum.

$$b_{r,i}^{(s,S)}(t_n) = \begin{cases} S - I_i(t_{n-1}), & \text{if } I_i(t_{n-1}) \leqslant s, \;\; S \leqslant L_i \\ 0, & \text{otherwise} \end{cases} \tag{4.2}$$

(s,S) inventory policies are useful for bulk materials where the limiting factor is the capacity of feed material. For example, a bulk-material facility with a strict mass limit that is running at a high fraction of its maximum capacity.

4.5.2 Reorder point/reorder quantity - (R,Q)

In a (R,Q) inventory policy, the minimum value R functions similarly to the minimum s value in an (s,S) policy [108]. However, the amount to order is always the same fixed quantity, Q. Equation 4.3 gives the demand request $b_{r,i}(t_n)$ for an (R,Q) inventory policy at time step t_n.

$$b_{r,i}^{(s,S)}(t_n) = \begin{cases} Q, & \text{if } I_i(t-1) \leqslant R,\ \ (Q + I_i(t-1)) \leqslant L_i \\ 0, & \text{otherwise} \end{cases} \tag{4.3}$$

(R,Q) inventory policies are useful when the transportation of an agent's incoming feed material is restricted to a known mass. For example, spent fuel transportation casks hold a specific number of assemblies. A reprocessing plant should receive an integer number of casks at once, whose total mass could be represented well by Q.

Table 4.2 and Figure 4.7 compare these two new inventory policies to the default inventory management behavior. The lower bound is 2 and the upper bound is 12, that is $s = R = 2$ and $S = Q = 12$. The maximum inventory size is only applicable to the default case, and is $L_i = 12$.

At each time step, the previous time step's inventory is reviewed and the agent places a request $b_{r,i}$. In this example the request is always fulfilled.

Some material is outgoing for downstream usage. The downstream desire is based on the same pseudo-random sequence $z(t)$ across all three cases. The amount of material that actually leaves the buffer is set by the supply constraint, $b_{s,i} = \min\left(I(t_{n-1}),\ z(t_n)\right)$. Thus, the inventory at the end of time step t_n is

$$I_i(t_n) = I_i(t_{n-1}) + b_{r,i} - b_{s,i} \tag{4.4}$$

In Figure 4.7, the black line shows the inventory in the agent across the default behavior, along with (R,Q) and (s,S) policies. The incoming material, equal to $b_{r,i}$, and outgoing material, equal to $b_{s,i}$, are the positive blue and negative yellow bars, respectively.

Table 4.2: Comparing (s,S) and (R,Q) inventory management

Time		0	1	2	3	4	5	6	7
Outgoing request ($z(t)$)		1.26	2.61	1.09	3.17	4.13	4.22	1.97	2.93
Incoming ($b_{r,i}$)	default	12	0	2.61	1.09	3.17	4.13	4.22	1.97
	(s,S)	12	0	0	0	0	11.00	0	0
	(R,Q)	12	0	0	0	0	12.00	0	0
Outgoing ($b_{s,i}$)	default	0	2.61	1.09	3.17	4.13	4.22	1.97	2.93
	(s,S)	0	2.61	1.09	3.17	4.13	1.00	1.97	2.93
	(R,Q)	0	2.61	1.09	3.17	4.13	1.00	1.97	2.93
Inventory ($I_i(t)$)	default	12	9.39	10.91	8.83	7.87	7.78	10.03	9.07
	(s,S)	12	9.39	8.30	5.13	1.00	11.00	9.03	6.06
	(R,Q)	12	9.39	8.30	5.13	1.00	12.00	10.03	7.06
Space available (L_i)	default	0	2.61	1.09	3.17	4.13	4.22	1.97	2.93
	(s,S)	0	2.61	3.7	6.87	11.00	1.00	2.97	5.94
	(R,Q)	0	2.61	3.7	6.87	11.00	0.00	3.97	6.94

The default behavior results in small requests at every time step using the request function given in Equation 4.1. Both (s,S) and (R,Q) policies order larger quantities less frequently using the request functions from Equations 4.2-4.3.

The subtle difference between an (R,Q) and (s,S) inventory policy can be seen at time t_5 and beyond. In both cases, the inventory from the previous time step is $I_i(t_4) = 1.00$. This is below the minimum threshold for both policies, allowing the agent to request new material at t_5.

Under (R,Q), the request for new material is always $Q = 12.00$. For (s,S) the request is $S - I_{t_4} = 11.00$. In both cases, both policies receive their requested amount. The two policies continue to diverge in time step 8, where the lower maximum value of the (s,S) policy results in dropping below the reorder threshold a time step ahead of (R,Q). The use of the two policies can be distinguished by whether the agent,

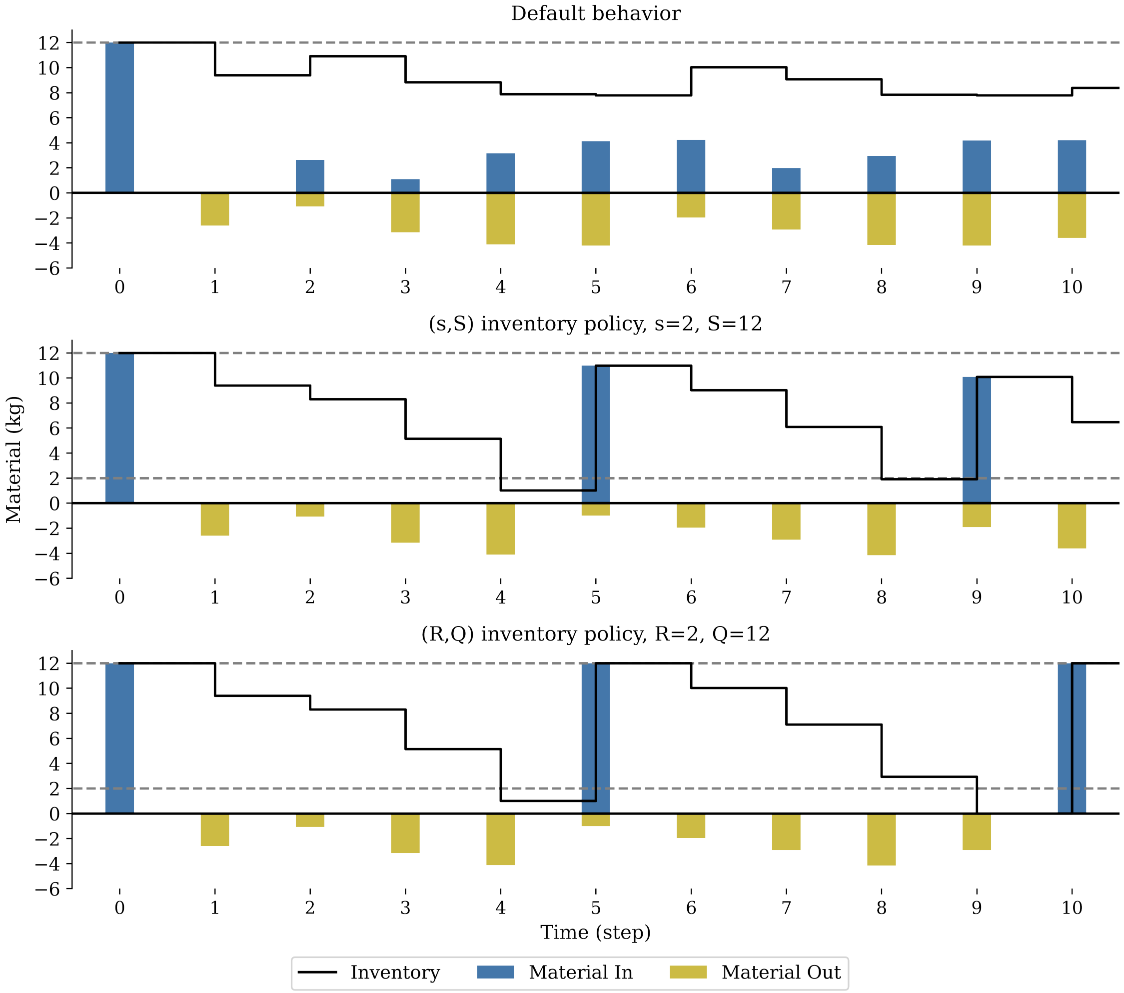


Figure 4.7: (s,S) policy and an (R,Q) policy using the same parameters and sequence of random numbers reducing (buying) the inventory. $s = R = 2$, *and* $S = Q = 12$.

after buying, should end up with at least the upper bound of material or no more than the upper bound. An (R,Q) inventory policy will always end up with at least Q inventory after buying (but no more than $Q + R$), while an (s,S) policy will never end up with more than S in the inventory.

4.5.3 Cumulative capacity-based inventory

The final continuous review inventory policy stays active until a cumulative amount of incoming material is received and then enters a dormant period.

This policy is motivated by the desire to model fresh fuel vaults. The default behavior of `Cycamore:Storage` causes the fresh fuel vault to seek a new batch of nuclear fuel immediately after the current batch is loaded into the reactor, instead of near the end of the following cycle.

Realistically, fresh fuel vault agents should not maintain any inventory over the long term but should be able to pass through relatively large quantities of material at the right time and then remain dormant until called upon again.

When modeling a fresh fuel vault, there should be no demand for new fuel during most of an operational cycle. Plant operators do not want their next cycle's new fuel at the beginning of the previous cycle, as it would generate no value for many months or years until the next refueling outage. Therefore, its inventory policy should support zero inventory and zero demand for a certain length of time.

A fresh fuel vault should seek exactly one batch worth of material during an active phase. Regardless of how long it takes to acquire this material, the fresh fuel vault should maintain the demand until enough material is available to fuel the core. After a full batch is obtained, the fresh fuel vault should undergo a dormant period until the next cycle is about to begin. The dormant phase is well-modeled using the time-based dormant tools described in Section 4.3.

The cumulative cap inventory policy was designed to allow the active cycle to be set by a total cumulative mass of material to be received. Regardless of whether the mass is received in one time step or one thousand, the agent will continue to request material until it has met its cap. Then, the agent will enter a dormant period

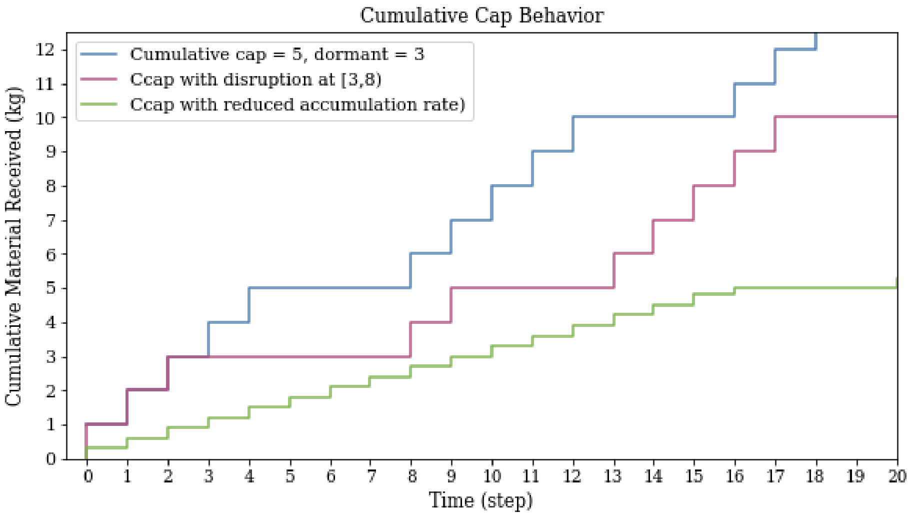


Figure 4.8: Cumulative cap policy with a cap of 5 and dormant period of three time steps in three different scenarios

immediately upon reaching the cumulative mass goal of the active period.

See Figure 4.8 for a demonstration of this policy with three scenarios with a cap of 5 kg and a dormant period of three time steps. When feed material is always available at the amounts expected, the cumulative cap policy acts like a time-based active dormant policy; in this case, there are five time steps of actively buying and then three dormant. In the second scenario, no material was available to the agent between time steps three and eight. The agent continues to seek the final two kg, delaying the start of its dormant phase. In the third scenario, the agent takes as long as needed to reach the cap when receiving less material than its maximum request.

A cumulative cap inventory policy is useful whenever materials should be ordered on a cyclic basic, but the active phase is better represented by a quantity of feed material to order rather than an expected length of time.

4.6 Packaging

Packaging takes unrestricted amounts of nuclear material and splits or merges it into distinct packaged materials based on mass limits and filling strategies. Each packaged item represents a physically meaningful object, such as a fuel assembly or a sample container, that is tracked and recorded separately from any other item. Transport units are a layer on top of packaging that link together multiple itemized packages, such as requiring four items, perhaps enriched UF_6 cylinders, to be shipped together as a set, such as being on a flatrack.

Packages are integrated into the Material Sell Policy to restrict the way that agents can offer material to the DRE to mimic the realistic behavior of nuclear material packaging and transportation containers.

4.6.1 Conceptual overview of packages

Packaging in Cyclus is a restriction placed on the form of nuclear materials as they move between facilities. Packaging may be used to aid agents in their processing of nuclear material based on other physical attributes that do not necessarily flow down from the physical aspects of transporting nuclear material but rather flow down from the design of a facility, such as tanks, pipe flows, or storage drums.

Package types have three parameters in addition to a unique name. The parameters are a fill minimum P_i^{min}, a fill maximum P_i^{max}, and a filling strategy $P_i^{strategy}$.

Table 4.3: Package parameters

Parameter	Type	Description
P_i	string	Package of name i
P_i^{min}	double	Fill minimum for package i
P_i^{max}	double	Fill maximum for package i
$P_i^{strategy}$	string	Filling strategy $\in$ {first, equal, uniform, normal}

A resource can be described as one of several types based on its package, as described in Table 4.4. If no user-defined package types are applied to a resource, it has default packaging type `unpackaged`, which can be called unpackaged bulk. There are no restrictions on the material quantity. If a packaging type is applied, it is either packaged bulk or as an item. Items have a fixed mass, $P_i^{min} = P_i^{max}$, otherwise they are packaged bulk because two items of the same package could have different masses.

Items are used to represent objects where the manufacturing tolerance is small enough that every item can be considered to have the same mass, such as fuel assemblies and bundles.

Table 4.4: Resource type by packaging parameters

Type	Description
Unpackaged bulk	No restrictions
Packaged bulk	$P_i^{min} < P_i^{max}$
Item	$P_i^{max} - P_i^{min} < \epsilon$

When packaged bulk is used, the filling strategy determines how packages will be filled. Strategy “first” fills up each package sequentially to P_i^{max}, filling one partial package at the end if the remaining material is above P_i^{min}. Strategy “equal” attempts to find a single average mass such that all material is shipped in an integer number of packages with no leftovers. Strategies “normal” and “uniform” are stochastic, sampling from a distribution created from the P_i^{min} and P_i^{max} to determine the fill mass m of each package.

4.6.2 Package implementation in Cyclus

Package type is a permanent parameter of resources. All resources must be assigned a package at creation or will be given the default `unpackaged` package. From every

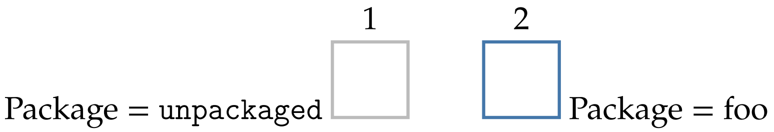


Figure 4.9: All resources, shown as rectangles, have a packaging type denoted by their line color. The default packaging type is unpackaged

time after creation, resources have a package type, either `unpackaged` or a user-defined package. Resources can be repackaged at any time, including through splitting and merging to comply with new package restrictions.

4.6.2.1 Filling Strategies

The simplest way of designing a package is an item with a fixed mass value. In this case, the filling strategy is not consulted because either packages will be filled or not.

In any other case, a packaged resource represents a bulk item, where it is possible that items could have a range of fill masses. When the product buffer has an inventory $I(t_n) > P_i^{max}$ of material, the filling strategy is used to determine how much mass is to be placed in each of the j packages that can be filled, up to a total of $M = \sum_{i=0}^{j} m_o \leqslant I(t_n)$. Note that agents may have multiple resource buffers, the inventory $I(t_n)$ used here specifically refers to the product buffer where material is ready to be traded to another agent.

The simplest filling strategy is "first", shown in Algorithm 1, which simply fills up packages to P_i^{max} until the remaining inventory has less than the P_i^{min} worth of resources. In the following algorithms, j is the number of packages, I is the inventory available, P_i^{min}/P_i^{max} are the fill limits, and m_j is the package fill mass for package j.

The other deterministic strategy is "equal" which attempts to find a single mass in between P_i^{min} and P_i^{max} that maximizes the amount of material that can be packaged.

Algorithm 1 Packaging fill strategy - first

```
$j \leftarrow 0$
while $I(t_n) \geqslant P_i^{min}$ do
    if $I(t_n) \geqslant P_i^{max}$ then
        $m_j \leftarrow P_i^{max}$
    else
        $m_j \leftarrow I(t_n)$
    $I(t_n) \leftarrow I(t_n) - m_j$
    $j \mathrel{+}= 1$
return $I(t_n), m_0 \cdots m_j$
```

In the case that there is no solution below P_i^{max}, then the available material cannot be packaged with a single mass, as shown in Algorithm 2.

The equal strategy determines how many packages could be filled at a mass of P_i^{min} by taking the floor of the available product divided by the P_i^{min}, $\lfloor I/P_i^{min} \rfloor$. This is the upper limit of how many packages could actually be filled.

How many packages could potentially be filled at a mass up to P_i^{max} is determined by taking the ceiling of the available product by P_i^{max}, $\lceil I/P_i^{max} \rceil$.

If the number of packages at P_i^{min} is equal to or above the ceiling of the number of packages at P_i^{max}, then there is a solution for a single mass that can be used to fill an integer number of packages with none remaining. If not, then there is no single fill mass across an integer number of packages that can leave no material remaining. In that case, the strategy defaults to "first" where packages are filled to P_i^{max}.

For example, consider a package type with $P^{min} = 2$ and $P^{max} = 3$. If the available inventory is $I = 3.5$, there is no solution that can package all the available inventory. In this case, the strategy defaults back to a "first" strategy where as many packages as possible are filled to P^{max}, and the remaining inventory does not get packaged. In this case, $M = \sum_{i=1}^{1} m_i = m_1 = 3$.

Among the deterministic filling strategies, "equal" is more efficient at packaging

Algorithm 2 Packaging fill strategy - equal

```
$j \leftarrow 0$
$n_{\text{at fill min}} \leftarrow \lfloor I(t_n)/P_i^{\min} \rfloor$
$n_{\text{up to fill max}} \leftarrow \lceil I(t_n)/P_i^{\max} \rceil$
if $n_{\text{at fill min}} \geqslant n_{\text{up to fill max}}$ then
    $m \leftarrow I(t_n)/n_{\text{up to fill max}}$
else
    $m \leftarrow P_i^{\max}$
while $I(t_n) \geqslant P_i^{\min}$ do
    if $I(t_n) \geqslant m$ then
        $m_j \leftarrow m$
    else
        $m_j \leftarrow I(t_n)$
    $I(t_n) \leftarrow I(t_n) - m_j$
    $j += 1$
return $I(t_n), m_0 \cdots m_j$
```

material than "first". Figure 4.10 shows this discrepancy for a simulation with a source that applies packaging with $P^{\min} = 0.75$, $P^{\max} = 1.25$. The histograms include the packages filled over the course of 10,000 time steps.

Another agent places a request b_r for the available product, with the value of the request sampled at each time step from a distribution $N(\mu = 2, \sigma = 0.25, a = 0, b = 2.5)$. While the "equal" strategy is always able to create two packages because the maximum allowed demand is exactly 2 $P^{\max}$, the "first" strategy is only able to trade two packages when the sampled demand is greater than $P^{\min} + P^{\max} = 2$, or the upper half of the normal distribution, otherwise a single package of $P^{\max}$ is traded.

There are two stochastic filling strategies, a uniform distribution and a normal distribution. The distributions are generated automatically from the packaging $P_i^{\min}$ and maximum. The uniform strategy samples from a continuous uniform distribution between the minimum and maximum. The normal distribution is created with a mean in the middle of the $P_i^{\min}$ and $P_i^{\max}$ and is three standard deviations in each

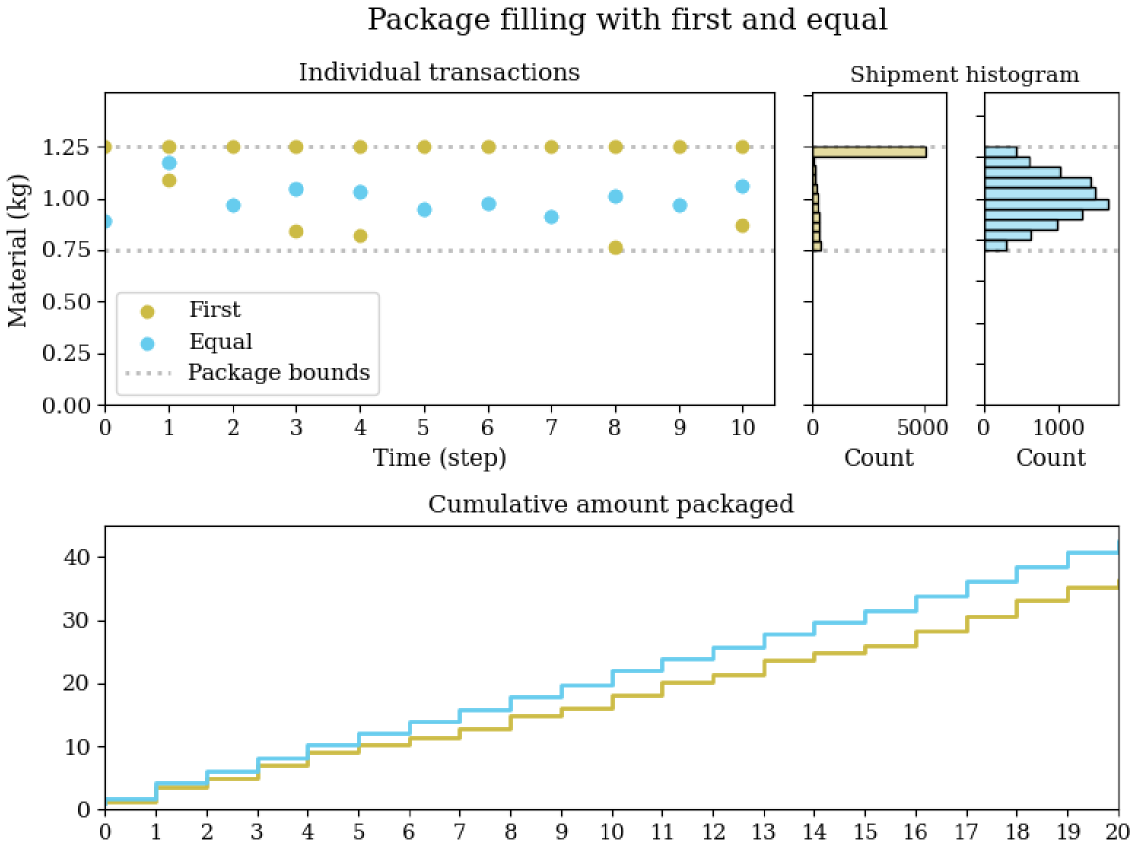


Figure 4.10: Strategy "first" is less efficient than "equal". When all other parameters are fixed, a packaging "first" strategy will be able to ship less material over time.

direction to the truncation points, also the P_i^{min} and P_i^{max}. Algorithm 3 describes the strategy implementation for both normal and uniform distributions.

When less than one P_i^{max} but more than the P_i^{min} is available, sampling of the distribution is bypassed because only part of the distribution would represent a valid fill, which would cause a skewed distribution over time. In this case, the total available inventory becomes the package fill, $m_j = I(t_n)$.

$$U(a = P^{min}, b = P^{max}) \tag{4.5}$$

$$N\left(\mu = \left(\frac{P^{max} + P^{min}}{2}\right), \sigma = \left(\frac{P^{max} - P^{min}}{6}\right), a = P^{min}, b = P^{max}\right) \tag{4.6}$$

Algorithm 3 Packaging fill strategy - normal or uniform

```
$j \leftarrow 0$
while $I(t_n) \geqslant P_i^{max}$ do
    $m_j \sim U_i(a, b)/N_i(\mu, \sigma, a, b)$
    $I(t_n) \leftarrow I(t_n) - m_j$
    $j \mathrel{+}= 1$
if $I(t_n) \geqslant P_i^{min}$ then
    $m_j \leftarrow I(t_n)$
return $I(t_n), m_0 \cdots m_j$
```

Figure 4.11 shows the distribution of m over the course of 10,000 time steps for strategies “uniform” and “normal”, with the same simulation parameters used in Figure 4.10.

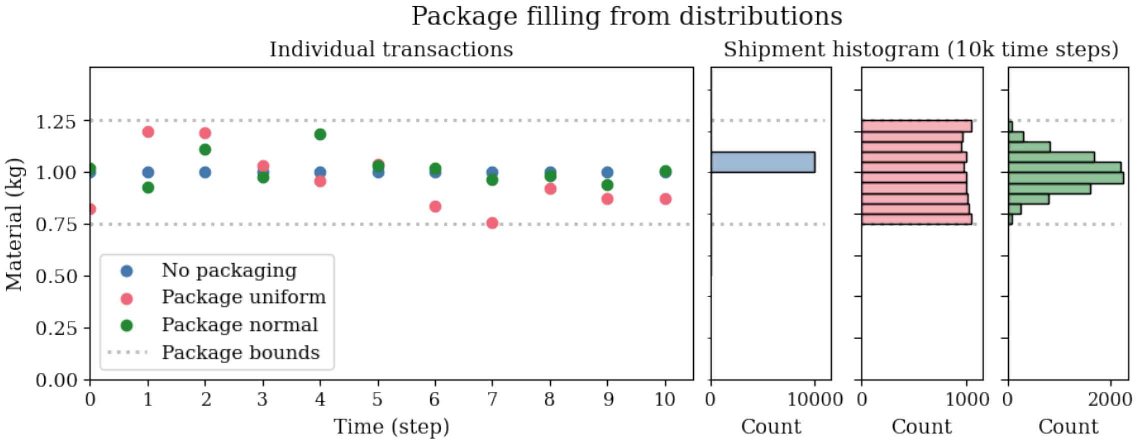


Figure 4.11: Stochastic package filling strategies, normal and uniform

Before packaging was added, an agent would have product available to trade based on the amount of feed material that could be processed per time step, if there were no resource constraints. This amount, the maximum throughput h_{max}, would typically equal the trade size if another agent continuously requested the product commodity. If an agent could produce 100 kg of a product per time step, then trades were typically 100 kg.

When the expected value of a stochastic filling strategy is used with the same expected value as the throughput $h_{i,max}$ in an agent without packaging, the same amount of material will be available as the time steps become large, if all other parameters remain equal. This allows the stochastic packaging strategies to be deployed in way that introduces natural variation in bulk materials while allowing the same cumulative material movement through the agent.

4.6.2.2 Packaging in the Material Sell Policy

Package type is a core parameter of a resource in CYCLUS, but packages are not separate physical items from the materials they contain. In the real world, UF_6 cylinders are individual objects, each with a tracking number. They exist regardless of whether they are filled with nuclear material. Packages in CYCLUS are conversely just a restriction and a parameter tied to each resource. All instances of a package type are identical, and there can be an unlimited number of each package type.

The use of packages and packaging processes could be applied at any point in an archetype. They are demonstrated here as part of the selling side of the DRE. Similar to how all of the buy or demand side parameters introduced above were placed within the CYCLUS toolkit in the Material Buy Policy, packaging capabilities have been placed in the CYCLUS toolkit in the Material Sell Policy and are available to all archetypes that use the Material Sell Policy.

When a Material Sell Policy is initiated by an agent, it is initiated with an outgoing package type i, where i has been declared in the input file. In the DRE, requesting agents first request material in the Request for Bids (RFB) phase [99]. These requests are for a quantity of a specific commodity and can have associated parameters such as isotopic composition. Then, in the Response to Request for Bids (RRFB) all agents can review the requests and place bids for material they could provide. A supplying agent makes bids on all commodities it could supply, up to the maximum quantity that could be supplied for each requester.

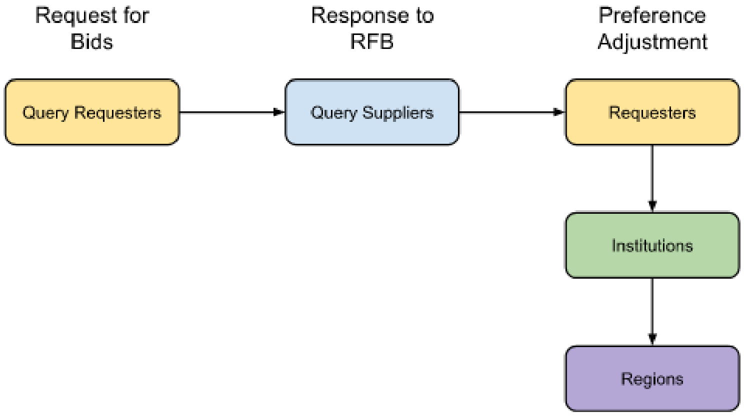


Fig. 2. Schematic illustrating the DRE's information gathering phases: Request for Bids (RFB), Response to Request for Bids (RRFB), and Preference Adjustment (PA).

Figure 4.12: Dynamic Resource Exchange overview [99]

An agent with a Material Sell Policy initiated with packaging will incorporate packaging strategies into its response to requests for bids. Assume for all further discussion that the commodities match between the requesting agent and supplying agent.

When making a bid at time t_n to respond to a request $b_{r,j}$ from another agent j, the supplying agent i considers its inventory currently available to trade at time t_n, $I(t_n)$, and calculates (the packaging analysis is always limited by the inventory or the demand, whichever is smaller) its packaged mass m based on the strategies described above. C is the maximum amount that agent i could satisfy before considering packaging. The agent responds as a supplier with constraining value

$b_{s,i}$.

$$C = \min(b_{r,j}, I_i(t_n)) \tag{4.7}$$

$$b_{s,i} = \begin{cases} \{m_k\} \forall k \in \{1 \cdot \cdot \lfloor \frac{C}{m} \rfloor\} + (C \mod m), & \text{if } (C \mod m) \geqslant P_i^{min} \\ \{m_k\} \forall k \in \{1 \cdot \cdot \lfloor \frac{C}{m} \rfloor\}, & \text{otherwise} \end{cases} \tag{4.8}$$

An agent may offer up to $\lfloor C/m \rfloor$ bids of size m, plus up to one bid of smaller size if the remaining inventory is still above the package minimum, that is if $(C \mod m) \geqslant P_i^{min}$.

4.6.3 Uses

One of the benefits of packaging resources to be shipped between agents, or in any part of the system, is the ability to track nuclear materials in a way that approximates real nuclear material accounting. This capability is essential for the use of system-scale fuel cycle modeling for international safeguards or nuclear security applications. As described in Chapter 5, the physical packaged unit of nuclear material is the accountable unit.

Another common usage of packaging is to limit agents with small throughput h from sending unrealistically small amounts of material each time step. Consider a simple system with one unit of material made available for trading each time step. The default behavior of an agent would offer that material to the DRE each time step. If the item package with $P_i^{min} = P_i^{max} = 4$ is applied, the agent will instead offer one package of four units every four time steps, as shown in Figure 4.13. When the regular flow of materials is periodically divisible into filled packages, packaging does not impede the flow of nuclear materials through the system. As $t_n \to \infty$, the packaging agent ships material at the same rate on average as the agent that offers its full inventory each time step.

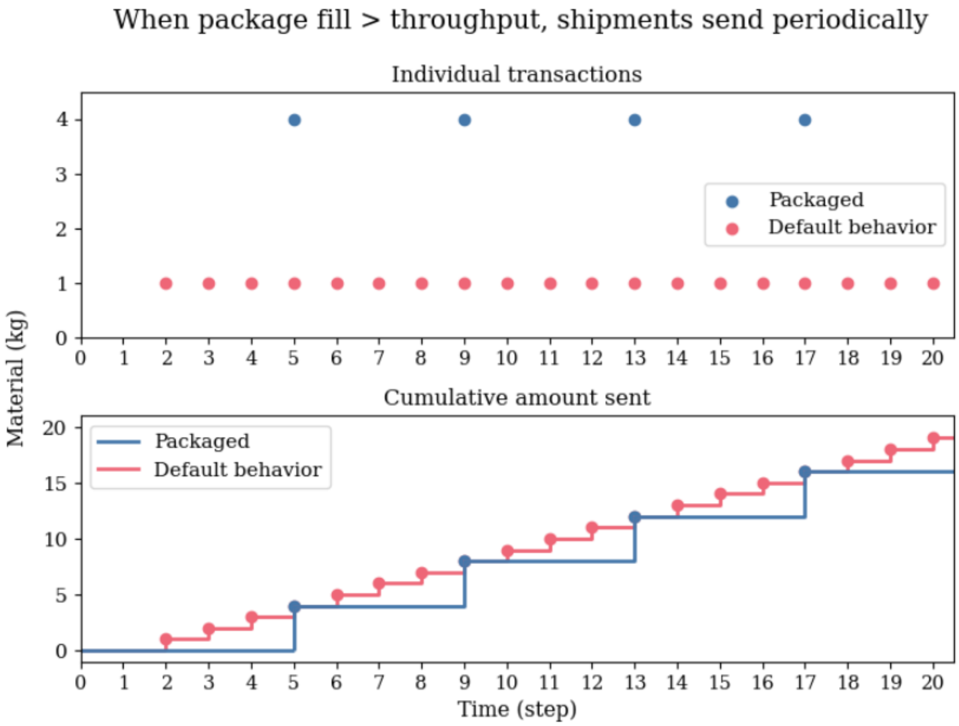


Figure 4.13: When the inventory flow into an agent is fully divisible into packages, the total amount shipped can be the same as when packaging is not employed

Packaging can impede a system when the maximum inventory of the packaging agent is not fully divisible into packages, as when Condition 4.9 is true, or when h is not divisible into packages (when Condition 4.10 is true). Both scenarios also require the packaging agent or any upstream agent to have and reach inventory limitations.

$$\left\lfloor \frac{L_i}{P_i^{min}} \right\rfloor < \left\lceil \frac{L_i}{P_i^{max}} \right\rceil \tag{4.9}$$

$$\left\lceil h_i \cdot P_i^{min} \right\rceil > P_i^{min} \tag{4.10}$$

Both scenarios result in the packaging agent having a time step in the packaging cycle where the material shipped is less than $h_{i,max}$. This slows the system down in an irrecoverable way. Regardless of how long the simulation runs, the total amount shipped will never equal the default behavior simulation.

Consider a situation with an item package $P_i^{min} = P_i^{max} = 2.5$ with $L_i = 2.5$. In this case, Condition 4.10 is true, and the inventory limit is reached on the third time step of the packaging cycle, where the space available is less than the maximum possible throughput, $L_i - I_i(t) = 0.5 < h_{i,max}$.

Although $h_{i,max}$ is still 1 unit per timestep, the combined packaging and inventory restrictions result in an effective throughput $h_{i,eff} = {}^{2.5 \text{ units}}/_{3 \text{ time steps}}$, or 5/6 units per time step. Figure 4.14 shows the delay, which results in a reduced amount of material shipped over time compared to an agent without a packaging-throughput mismatch.

When materials are packaged by their supplier, the requesting agent may either retain the packaging or strip it once trades have been executed. Agents modeling chemical or nuclear processes are likely to strip packaging to further manipulate the material, but `Storage` agents, such as the receiver MBA of a larger facility or a storage-focused facility like consolidated interim storage (CIS), may retain the packaging type.

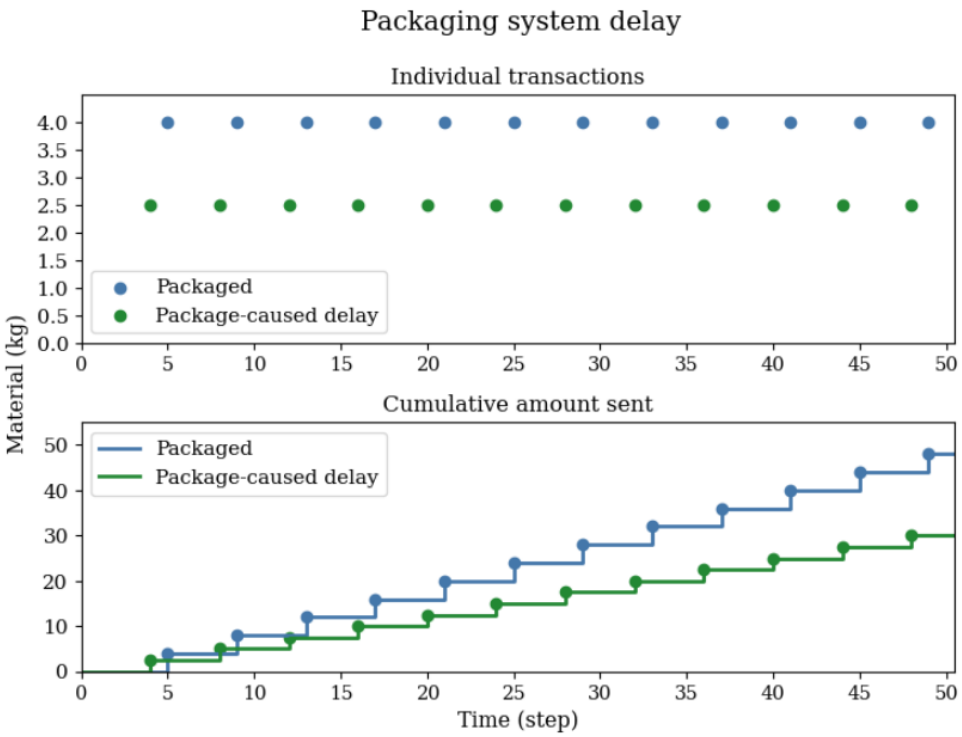


Figure 4.14: When inventories are not neatly divisible into packaging, causing inventory limits to be reached, permanent delays are introduced into the system

4.6.4 Conceptual overview of transport units

One more optional layer of packaging was added to the packaging process, called Transport Units TU. Packages are important, particularly in representing realistic nuclear material accounting of individual items, but the actual transport of nuclear material in the real world is further restricted by multiple packages being moved together as a unit or a grouping in between facilities. These groupings are applicable across the fuel cycle; for example, around 36 drums fit in a 20-foot shipping container (depending on stowing and lashing procedures), up to four Type 30B UF_6 cylinders can be placed on a flat rack, and multi-purpose canisters can hold dozens of used fuel assemblies depending on manufacturer and fuel design that may be transported for both interim storage and to disposal facilities.

Transport units have three parameters. The parameters are a fill minimum TU_i^{min}, a fill maximum TU_i^{max}, and a filling strategy $TU_i^{strategy}$.

Parameter	Type	Description
TU_i	string	Transport unit with name i
TU_i^{min}	integer	Fill minimum for transport unit i
TU_i^{max}	integer	Fill maximum for transport unit i
$TU_i^{strategy}$	string	Filling strategy $\in$ {first, equal, hybrid}

Table 4.5: Transport unit parameters

Transport units also have filling strategies first and equal, but also a hybrid strategy. Hybrid attempts to fill transport units to their maximum fill but calculates whether near the end of the filling process an equal strategy would prevent leftover material. The hybrid strategy is implemented because transport units handle only integer numbers of packages, rather than positive real numbers that must be filled for packages.

4.6.5 Transport Unit implementation

Transport units, unlike packages, are not implemented into CYCLUS as a fundamental property of a resource. Instead, transport units are just a method that can be used to further restrict the movement of packaged materials in a realistic manner. Another fundamental difference between packages and transport units is that packages can be filled with any amount of nuclear material, but transport units are integer quantities of packages.

Transport units are declared like packages, as an optional, repeatable block in a CYCLUS input file. Also like packages, archetypes that use transport units must pull from the simulation-wide list of transport units, they should not be declared directly in an prototype (facility) block.

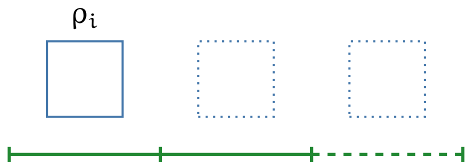


Figure 4.15: Transport units are not a parameter of resources, but are applied to groups of resources. Restrictions are shown as a line below resource boxes. In this case, TU^i_{min} *is the solid line at 2 resources, and* TU^i_{max} *is the dotted line at 3 resources. Dotted boxes show missing resources.*

Consider a situation where one package is available, the transport unit minimum is two, and the maximum is three. This is shown in Figure 4.15. One package cannot be shipped as a transport unit by any filling strategy, so zero packages are available to offer. Two or three packages would be shippable, and four could be shippable depending on the filling strategy.

4.6.5.1 Filling strategies

Transport units have filling strategies "first" and "equal", similar to packaging but based on integer quantities and rounding rather than floats. These strategies are described in Algorithm 4 and Algorithm 5 and use the same logic, except using integers instead of real numbers. The number of packages available is P, the transport unit fill is q, and the total shippable packages is Q.

Algorithm 4 Transport unit maximum shippable packages - first

```
$Q \leftarrow 0$
$q \leftarrow 0$
if $P \geqslant TU_i^{max}$ then
    $q \leftarrow TU_i^{max}$
else if $P \geqslant TU_i^{min}$ then
    $q \leftarrow P$
$Q \leftarrow \min\left(P,\ q * \frac{P}{q}\right)$
return $Q$
```

This layer also has a "hybrid" iterative strategy, as described in Algorithm 6.

Algorithm 5 Transport unit maximum shippable packages - equal

```
$Q \leftarrow 0$
$q \leftarrow 0$
if $P \geqslant TU_i^{max}$ then
    if $\lfloor (P/TU_i^{min} \rfloor \geqslant \lceil (P/TU_i^{max} \rceil$ then
        $q \leftarrow \lfloor (P/n_{\text{at fill max}} \rfloor$
    else
        $q \leftarrow TU_i^{max}$
else if $P \geqslant TU_i^{min}$ then
    $q \leftarrow P$
$Q \leftarrow \min\left(P,\ q * \frac{P}{q}\right)$
return $Q$
```

The hybrid strategy, unlike first and equal, iteratively calculates the best fill for the next round of transport units. If the remaining number of packages could be filled equally with an amount less than the fill maximum but not at the fill maximum, then the strategy will fill packages at that mass, otherwise it will fill transport units to the maximum.

The hybrid strategy can avoid a common issue with the first and equal strategies, which occurs when the remaining packages to place in a transport unit are above the fill maximum and twice the minimum but below twice the maximum, $(TU_i^{max}, 2TU_i^{min}) < P < 2TU_i^{max}$.

Consider a situation with $P = 11$, $TU^{min} = 3$ and $TU^{max} = 4$. The first strategy will create transport units $Q = \{4, 4\}$ with 2 remaining packages. Only after filling the second transport unit with four packages would the first strategy recognize that the remaining packages are less than the minimum, and be unable to fill a third. The equal strategy will identify that no fixed number of packages, either three or four, would use all packages. Filling three packages of three, $Q = \{3, 3, 3\}$ leaves only one package remaining. However, the hybrid strategy recalculates package size similar to equal but iteratively, it will fill the first two packages with size three, and then the third with four, the only strategy to successfully place all packages in a transport unit, $Q = \{3, 3, 4\}$.

Algorithm 6 Transport unit maximum shippable packages - hybrid

```
$Q \leftarrow 0$
$q \leftarrow 0$
while $P \geqslant TU_i^{max}$ do
    if floor($P/TU_i^{min}$) $\geqslant$ ceil ($P/TU_i^{max}$) then
        $q \leftarrow$ floor($P/n_{\text{at fill max}}$)
    else
        $q \leftarrow TU_i^{max}$
    $Q \leftarrow Q + q$
    $P \leftarrow P - q$
if $P \geqslant TU_i^{min}$ then
    $Q \leftarrow Q + P$
return $j$
```

As opposed to packages, transport units are not actually filled in any real way in the simulation. Resources are not split and merged, and no resource parameters are affected by transport units. Currently, transport units are only implemented as a go-no go check in the RRFB and trade execution steps of the DRE, as described in Section 4.6.5.2.

Current transport unit algorithms are not integrated with package filling algorithms. Packaging must be done first from the inventory mass $I(t_n)$ to obtain the number of packages of type i and P_i, then fed into the transport unit process. The output of the transport unit evaluation is the maximum number of packages that can be shipped.

4.6.5.2 Transport Units in the Material Sell Policy

Transport units have been demonstrated in the CYCLUS toolkit as part of the Material Sell Policy in conjunction with packaging. After the check on packaging is applied to confirm the number of bids (individual packageable amounts of material), then the total number of bids is checked against transport unit restrictions.

For example, consider a situation with five units of material and an item based package with $P^{min} = P^{max} = 1$ unit. The transport unit restrictions are that exactly three packages must be transported together, $TU^{min} = TU^{max} = 3$. Even though it would be possible to package all all five units into five packages, only three units of material are shippable with the combined packaging and transport restrictions. Therefore three units are bidded out to the DRE.

Note that the sequential nature of creating packages and then checking transport units raises the potential for failed trades due to restrictions, and inefficient trades are also possible.

4.6.6 Limitations

Packaging as implemented in the Material Sell policy has the potential to result in trades that cannot be executed because the requester accepts a partial bid. At the RRFB step, bids are just promises that material can be packaged if the bid is accepted by the requesting agent. No packaging is done at this step because there is no guarantee that any trades will be executed. If the requesting agent ultimately accepts a partial bid, (i.e. $\leqslant b_s$), there is no longer a guarantee that some or all of the partial amount will be packageable.

After the DRE has executed and optimized trades have been determined, then the supplying agent will attempt to package the accepted trades. If the inventory already has the outgoing package type, for example if the material was unpackaged and no outgoing packaging type was set, then nothing needs to happen. As an example, consider an agent that has $I_i(t) = 10$ units of material and has item-based packaging restrictions, $P_i^{min} = P_i^{max} = 4$ units. Although the request from agent j could be $b_{s,j} = 10$ units, the agent is not able to offer up all ten of its units. Packaging restrictions only allow inventory to be traded as one package of four units, or two packages for a total of eight units. In this case, the supplying agent will offer up eight units to the DRE, $b_s = \sum\{4, 4\} = 8$.

If the outgoing packaging is different than the existing packaging, then the material will be split or merged as necessary to achieve the packaging mass. Given the previous example, if both bids of four units each were accepted, then the agent will split off four units and four units from its inventory, packaging them and sending them off to the requesting agent as shown in Figure 4.16.

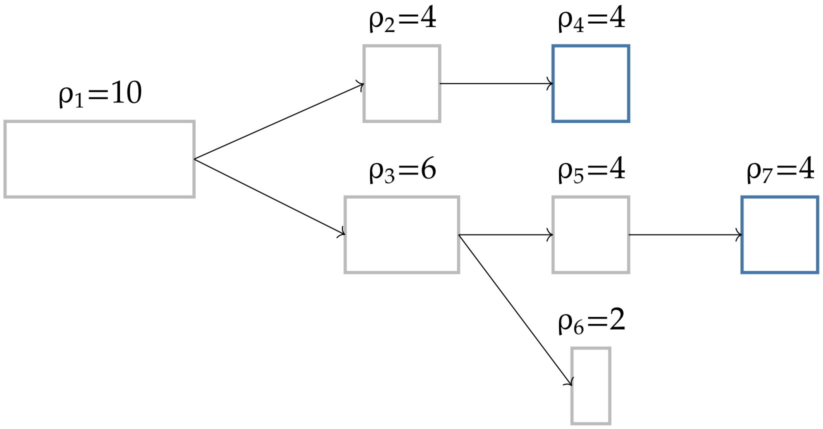


Figure 4.16: A resource tree for an agent splitting an inventory of size 10 to trade. Given the packaging restrictions, ρ_1 can only create two packaged resources of size 4, and the remaining two units are not packageable, and thus not tradable, at this time.

This introduces the risk of a failed trade. Returning to the example, ten units of material were available, but they could only be packaged into eight units, representing two packages of four.

If the requesting agent finds this bid less attractive than another bid, the supplying agent may receive a partially accepted trade. Assuming another more preferable bid from agent k provided all but six units of the requested material, then the supplying agent would be left with two accepted trades of four units and two units, for a total of six units.

In this case, agent i would be unable to execute the full accepted amount. As Figure 4.17 shows, one trade of four units would be successfully split off and traded. The other trade, of which only two units were accepted, would be split off and then evaluated against the packaging restrictions. Two units are not packageable, and the trade fails. The supplying agent must send one trade of four packaged units and one "failed trade" of zero units to the requesting agent.

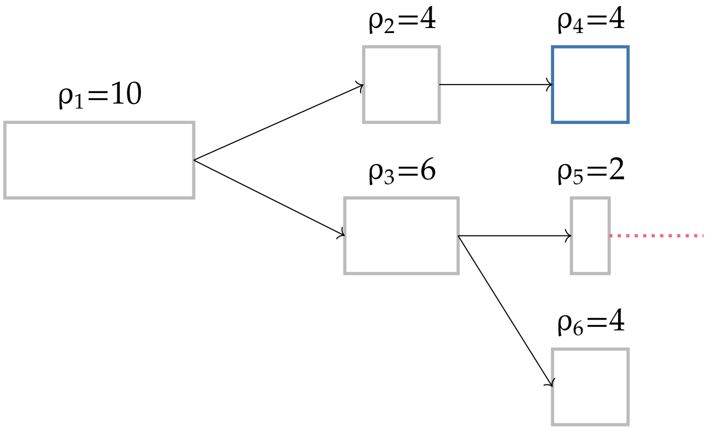


Figure 4.17: A resource tree for an agent splitting 10 units to trade. Given the packaging restrictions, a packaged resource (ρ_6) *of size two cannot be created from* ρ_3. *One of these two trades fails. Only* ρ_4 *will be sent to the supplier.*

In order to limit the number of failed trades, the bid information that goes to requesting agents during the preference adjustment phase (see Figure 4.12) can now include the packaging type that any accepted trades would be packaged into. While no agents currently make use of this information, it would be possible for requesting agents to confirm the packageability of possible trades, in the case that they intend to accept less than the full bid. Or, agents could simply consider bids that have associated packaging information as *exclusive*, as an all-or-nothing proposition.

If the requesting agent accepts a full bid sent by an agent using the Material Sell

Policy, it is guaranteed to package successfully because packaging restrictions are checked before the supplying agent participates in the RRFB.

Inefficient trades often occur with “first” strategies, which leave leftover material unpackaged because only the final package or transport unit can be partial-fill. Inefficiencies also occur when an “equal” packaging or transport unit strategy fills a large number of units near P_i^{min}/TU_i^{min} because the total amount isn’t all packageable near the maximum.

Similarly, package restrictions limit the ability to inject disruptions into the shipment process to study protracted diversion scenarios, where small amounts of material are repeatedly removed from nuclear materials over time, because there is not yet a way to override packaging restrictions.

The filling strategies for packages and transport units are a gross simplification of how real nuclear materials, especially bulk materials, get filled into real packages. Humans can override typical rules such as “fill to around 95% of regulatory limit" by filling partial packages if their customer requests it or by using separate packages like sample containers for requests of abnormal size.

4.7 Summary

This chapter introduced new tools for agents to control their request and supply of materials to replicate more realistic nuclear material movement patterns. Buying tools were added to the Cyclus toolkit’s Material Buy Policy and packaging was added to the Material Sell Policy, allowing any agent in the Cyclus ecosystem to easily leverage these new capabilities.

Active and dormant cycles, in Section 4.3, allow periodic behavior and are sampled from independent distributions. Inventory management tools in Section 4.5

allow agents' buying behavior to be set by either the inventory on hand, as in the (s,S) and (R,Q) policies, or by a cumulative mass received, as in cumulative capacity.

A PRNG and resource package type were added directly to Cyclus to support the new capabilities for the buy and sell policies, but can also be accessed by agents directly to support process modeling.

Packaging and transport units in the Material Sell Policy, described in Section 4.6, allow agents to restrict their supply of materials to realistic quantities based on fill limits and strategy.

5 SYNTHETIC NUCLEAR MATERIAL ACCOUNTING REPORTS

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The IAEA has an interest in improving the efficiency and timeliness of safeguards and using reproducible methods to limit the amount of expert judgments involved in safeguards analysis [109]. One area of potential improvement is in assessing nuclear material accounting reports, which present a wealth of detailed information. These reports are evaluated on a per-material balance area (MBA) level to assess trends in material unaccounted for (MUF) and other signatures of possible diversion, but there may be additional signatures of interest that can be identified from assessing trends and patterns across the entire fuel cycle, considered as an integrated system. This expansion of scope is aligned with the IAEA's State-Level Concept (SLC), which aims to integrate safeguards implementation and analysis across a State's entire facilities and capabilities. However, this type of research cannot be undertaken without access to real or realistic synthetic data on the order of an entire State.

Information about a State's inventory and movements of nuclear material is highly sensitive, both from a commercial perspective and from a security perspective. States and facility operators do not freely divulge this information, and the IAEA– which receives detailed information from States as accounting reports– considers all information concerning nuclear materials location and composition to be Safeguards Confidential. Even within the Agency, information marked as Safeguards Confidential can be accessed only on a direct need-to-know basis by those who analyze and summarize the information for that particular State. This restriction reflects of the sensitivity of granular information about nuclear material inventories and movements, and the gravity of facilitating the safeguards system described in Article III of the NPT.

For this reason, there have been few attempts to capture and comprehensively study nuclear materials on the State level. Previous research efforts using process or system-based nuclear fuel cycle simulation tools have focused on improving fidelity at the level of an individual facility, or even a single process. Because no actual data are available to researchers, fuel cycle simulations have either focused on simulating with very high temporal and spatial fidelity for one facility, or very low fidelity for long-term nuclear energy planning. The results of this project provide a new area of safeguards analysis by developing tools to generate synthetic data on nuclear material inventory, composition, and movements with safeguards-relevant spatial and temporal fidelity across an entire State's nuclear fuel cycle.

5.1 Nuclear material accounting reports

States with a comprehensive safeguards agreement (CSA) are obligated to develop a State system of accounting for and control of nuclear material (SSAC) , which defines how nuclear material accountancy is conducted and the resulting information reported to the IAEA. The exact details of safeguards implementation are negotiated between the State and the IAEA through Subsidiary Arrangements. These arrangements have a general part that applies to the entire State and FA that specifies the exact details of safeguards implementation for facilities and locations outside facilitiess (LOFs) in the State. Unlike CSAs, none of the information agreed upon in Subsidiary Arrangements becomes available to the public, unless a State chooses to divulge it.

This work follows the nuclear material accounting concepts and reporting structure recommended in the IAEA's Safeguards Implementation Practices Guide on Provision of Information to the IAEA (IAEA Services Series 33) [56] and in Model

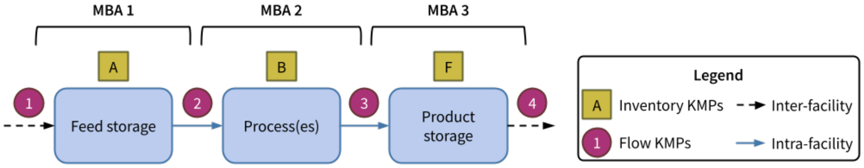


Figure 5.1: Notional three-MBA facility

Subsidiary Arrangements. Most notably, the 10th part, "Code 10 Contents, Format and Structure of Reports to the Agency", referred to as Code 10, details the reporting structure developed by the Agency [110].

Where available, model FAs will be used to determine the most realistic set of MBA(s) to represent a given type of nuclear facility, otherwise a notional three-MBA model will be used. The notional facility is shown in Figure 5.1, with a MBA1 for receipt of feed material, MBA2 for all chemical or nuclear processes, and MBA3 for storage of product and shipment to other facilities.

There are three versions of Code 10 that States may choose when deciding how to submit their regular accounting reports to the IAEA: labeled format, fixed format, and more recently, XML format; all contain the same information, each presented in a slightly different way.

There are three types of nuclear material accounting reports that must be submitted by each State: inventory change reports (ICRs), physical inventory listings (PILs), and MBRs. The ICR is a record of all transactions in all of a State's facilities under safeguards and represents the bulk of the State's reporting data. An ICR reports six primary processes:

1. Material enters MBA,
2. Material exits MBA,
3. Nuclear process changes to material within a MBA,
4. Re-batching changes the quantity of material tracked as a single unit,
5. Start of safeguards, and

6. Termination of safeguards.

Inventory changes must be reported within 30 days of the calendar month in which the change occurs, which effectively limits ICRs to contain one month's worth of information or less. ICR reports generated in this work are always one calendar month, varying from 28 to 31 days in length depending on the month.

PILs are, conversely, a snapshot of an MBA in time. With a frequency defined by its individual FA, often every 365 days, a PIL captures the inventory KMP, quantity, and composition of nuclear materials. The MBR is typically created at the same time as a PIL and contains summary information about the MBA since the last MBR report, including MUF and rounding adjustments. This work focuses on replicating the first of the three required State accounting report types, the ICR, in labeled format. ICRs are the largest fraction of nuclear material accounting reports and have the largest number of required labels per entry. Once ICRs have been replicated, the capability to generate PILs and MBRs would be a much simpler process. Much of the infrastructure needed to generate ICRs could be reused for the other two report types.

5.1.0.1 Bridging nuclear material structures with simulation agents

FAs are agreements concluded by a State and the IAEA and contain detailed information about a facility's design, safeguards measures, and accountancy. They include the precise breakdown of MBAs and KMPs for the facility, as well as the expected types of inventory changes to occur in the facility, and therefore factor heavily into how materials and their movements are recorded in accounting. Model FAs are often the basis or starting point for an agreement and propose standard MBAs and KMPs. However, these documents are not widely available to the general

R&D community. Where available, model FAs were used to determine the most realistic set of MBAs to represent a given type of nuclear facility, otherwise a notional three-MBA model is used, as in Figure 5.2.

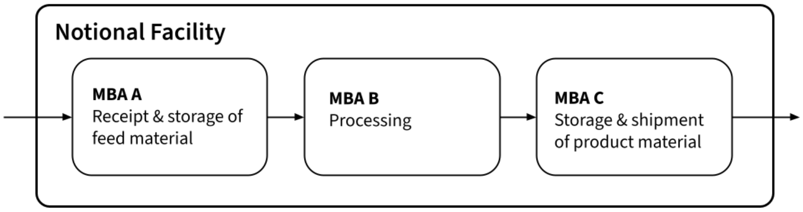


Figure 5.2: Notional three-MBA model for nuclear facilities

The data produced directly by nuclear fuel cycle simulators need additional processing to be reflected as synthetic nuclear material accounting data. In particular, there are areas where nuclear fuel cycle simulators produce too many data points, such as detailed accounting of mining and milling activities that are not covered under CSAs. The structures used to represent nuclear facilities for nuclear energy planning do not always correspond directly with core ideas such as MBAs, which are the fundamental spatial unit of IAEA nuclear material accounting.

This project addressed the issue of relevance in simulated data both by ensuring that extra data are removed, and by integrating FA information such as MBA and KMP codes to correctly partition simulation data.

This situation where two agents (discrete actors) belong to the same MBA requires that agents in a nuclear fuel cycle simulation never span more than one MBA. For example, Figure 5.3 shows two agents in the same MBA designation. In this case, any movements of nuclear material between the two agents will not be designated as an inventory change, and thus will remain invisible to the ICR. This can occur in reactors, where a fresh fuel vault, reactor, and UNF pool may all be represented by separate agents but are part of a single MBA, or in fuel cycle facilities where multiple agents are used to represent processes like pelletization and fuel rod-filling but are all within the process MBA.

On the other hand, the opposite is not possible. Data for one agent cannot be disaggregated to produce information for two MBAs.

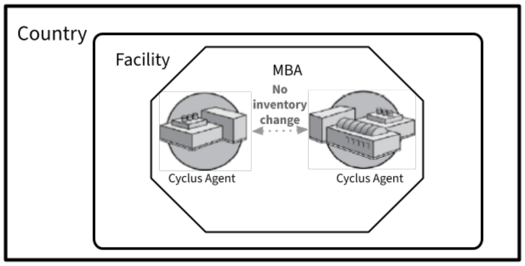


Figure 5.3: Two agents can belong to the same MBA

The Cyclus simulation output contains detailed information about the location, composition, and movement of nuclear materials throughout every agent in the simulation. The current version of Cntaur requires two additional user-input files that mimic information present in a FA in addition to a Cyclus simulation output.

The first file, referred to as the MBA file, links the agents or individual actors in the Cyclus world to the three relevant levels of information in an ICR: the country code, facility code, and MBA code. A Boolean parameter notes whether the agent should be used to generate accounting reports. This should be used to exclude facilities that are not required to submit detailed accounting reports under a CSA, such as mining and milling facilities, and any other agents that are ancillary and not representative of real and physical facilities. The second file, called the material description code (MDC) file, helps to link nuclear materials in Cyclus to a four-character code that contains information about the physical and chemical form.

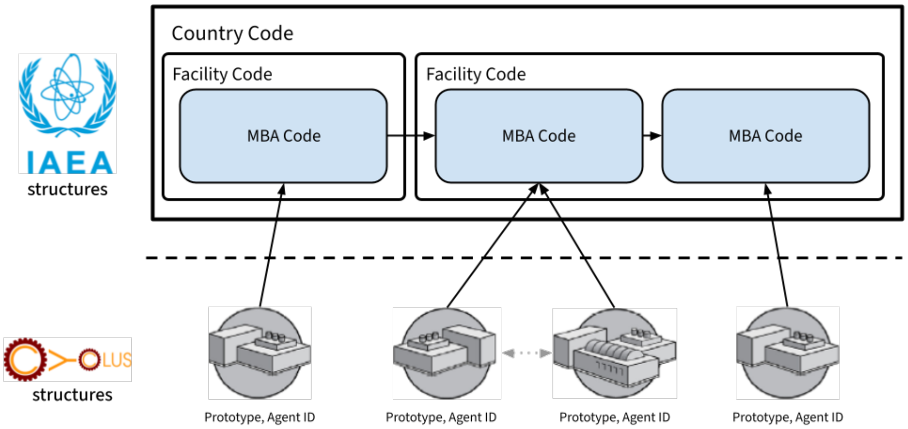


Figure 5.4: The MBA file links agents in a Cyclus simulation to its country, facility, and MBA code for accounting reports

5.2 Convert fuel cycle simulations to accounting reports

This project created a new computational tool, Cntaur, to convert Cyclus Nuclear simulations To state AccoUnting Reports. The tool generates ICRs, which require the generation of nearly all of the data elements specified in the Model Subsidiary Arrangements, General Part, Code 10 Contents, Format, and Structure of Reports to the Agency ("Code 10") [110].

Figure 5.5 shows the process of generating reports in Code 10 format for any nuclear fuel cycle that can be simulated using Cyclus. First, information should be gathered about a State's nuclear fuel cycle and other State-specific information. This information is combined into a Cyclus input file, and a simulation is run for the duration of interest. Because ICRs must include the exact date of an inventory change (412 Date of Inventory Change), simulations must run with a one-day (86,400-second) time step or shorter. If the fuel cycle being modeled has evolving facilities, the simulation can deploy and decommission new facilities at a specified

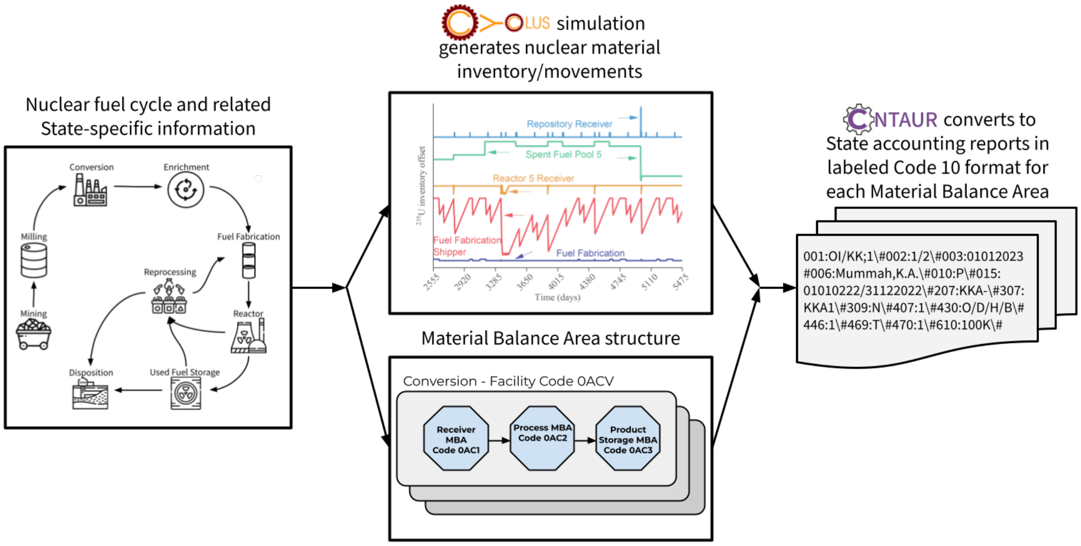


Figure 5.5: Process of generating simulated State accounting data

time step, or in response to an increased demand for more production capacity by the State.

Section 5.2.1 describes the Code 10 labels required to generate an ICR. Section 5.2.2 introduces the nuclear fuel cycle simulator Cyclus and details the development of Cntaur. Section 5.2.3 describes the process for a user to create synthetic Code 10 reports using Cntaur.

5.2.1 Code 10 labels replicated

Code 10 labels are the individual data fields that comprise an entry in a nuclear material accounting report. Labels are three digits long and many contain leading zeros. In this work, labels will be referred to by label number and description for ease of understanding, such as 307 MBA Code and 610 Natural Uranium. An entry on an ICR contains information about a single nuclear material movement or composition change. If at least one relevant movement or composition change happens within a single month, a report must be created from all the entries. A month with zero entries can be skipped.

The labeled format report is a string of labels, a delimiter, the label value, and a delimiter to end the value. The delimiters are specified in Table 5.1. A colon and a pound sign/hash are always included in an individual label and entry, and the other two values are used only when a value has multiple parts, such as in label 001 Reference Number, which has three separate components.

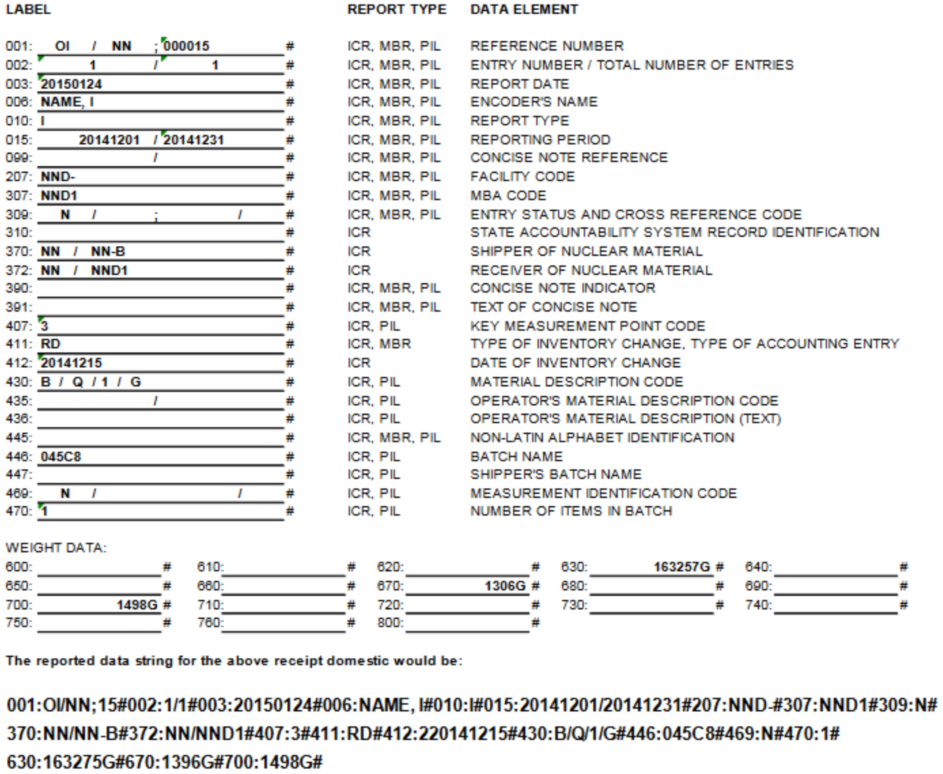
Table 5.1: Code 10 delimiters

Delimiter	Usage
:	Between the label and the value
/ ;	Separating multiple elements within a single value
#	Ending a value

Figure 5.6 shows how a labeled format report can be created from a more human-friendly table of labels by filling in the labels that apply to the particular entry and then combining them into a single string. Some entries are optional, such as 310 State Accountability System Record Identification and can be skipped if not relevant for a particular entry or report.

Required data elements can be categorized into four types: labels that can be generated directly from a Cyclus output file, labels that are fixed across all reports due to label features or Cyclus limitations, labels that can be generated from Cyclus simulation data plus additional user input, and labels that are not implemented at all.

Table 5.2 describes the main entries of an ICR that can be generated directly from Cyclus simulation output. Entries that deal with time, such as 015 Reporting Period and 412 Date of Inventory Change, can be determined directly from simulation time steps regardless if the simulation has a time step of one day. Commodity names and resource numbers can broadly be considered analogous to material descriptions



LABEL			REPORT TYPE	DATA ELEMENT
001:	OI / NN ; 000015	#	ICR, MBR, PIL	REFERENCE NUMBER
002:	1 / 1	#	ICR, MBR, PIL	ENTRY NUMBER / TOTAL NUMBER OF ENTRIES
003:	20150124	#	ICR, MBR, PIL	REPORT DATE
006:	NAME, I	#	ICR, MBR, PIL	ENCODER'S NAME
010:	I	#	ICR, MBR, PIL	REPORT TYPE
015:	20141201 / 20141231	#	ICR, MBR, PIL	REPORTING PERIOD
099:	/	#	ICR, MBR, PIL	CONCISE NOTE REFERENCE
207:	NND-	#	ICR, MBR, PIL	FACILITY CODE
307:	NND1	#	ICR, MBR, PIL	MBA CODE
309:	N / ; /	#	ICR, MBR, PIL	ENTRY STATUS AND CROSS REFERENCE CODE
310:		#	ICR	STATE ACCOUNTABILITY SYSTEM RECORD IDENTIFICATION
370:	NN / NN-B	#	ICR	SHIPPER OF NUCLEAR MATERIAL
372:	NN / NND1	#	ICR	RECEIVER OF NUCLEAR MATERIAL
390:		#	ICR, MBR, PIL	CONCISE NOTE INDICATOR
391:		#	ICR, MBR, PIL	TEXT OF CONCISE NOTE
407:	3	#	ICR, PIL	KEY MEASUREMENT POINT CODE
411:	RD	#	ICR, MBR	TYPE OF INVENTORY CHANGE, TYPE OF ACCOUNTING ENTRY
412:	20141215	#	ICR	DATE OF INVENTORY CHANGE
430:	B / Q / 1 / G	#	ICR, PIL	MATERIAL DESCRIPTION CODE
435:	/	#	ICR, PIL	OPERATOR'S MATERIAL DESCRIPTION CODE
436:		#	ICR, PIL	OPERATOR'S MATERIAL DESCRIPTION (TEXT)
445:		#	ICR, MBR, PIL	NON-LATIN ALPHABET IDENTIFICATION
446:	045C8	#	ICR, PIL	BATCH NAME
447:		#	ICR, PIL	SHIPPER'S BATCH NAME
469:	N / /	#	ICR, PIL	MEASUREMENT IDENTIFICATION CODE
470:	1	#	ICR, PIL	NUMBER OF ITEMS IN BATCH

WEIGHT DATA:

600:		#	610:		#	620:		#	630:	163257G	#	640:		#
650:		#	660:		#	670:	1306G	#	680:		#	690:		#
700:	1498G	#	710:		#	720:		#	730:		#	740:		#
750:		#	760:		#	800:		#						

The reported data string for the above receipt domestic would be:

001:OI/NN;15#002:1/1#003:20150124#006:NAME, I#010:I#015:20141201/20141231#207:NND-#307:NND1#309:N#
370:NN/NN-B#372:NN/NND1#407:3#411:RD#412:220141215#430:B/Q/1/G#446:045C8#469:N#470:1#
630:163275G#670:1396G#700:1498G#

Figure 5.6: Example of Code 10 labeled format. Image from IAEA

and batches.

Weight data are another key element of accounting reports that can be generated directly from Cyclus simulations; we have implemented the most commonly used labels. Most countries do not report weight data in terms of unified uranium, so Cntaur includes enrichment categories (depleted, natural, enriched), uranium-235 for enriched uranium, and other reportable nuclear materials as elements. Table 5.3 shows the individual weight data labels currently implemented.

For materials that meet the definition of NU or DU, no isotopic labels are required. Otherwise, if the ^{235}U content is above natural enrichment or ^{233}U is present, element label 630 Enriched Uranium plus the relevant fissile label is required. In most uranium-only fuel cycles, only label 670 ^{235}U is used. If ^{233}U is present in more than negligible quantities, such as a uranium-thorium fuel cycle, the combined fissile isotope label 660 ^{233}U + ^{235}U Isotopic Content is used. The use of this label occurs when a significant amount of ^{233}U is present, at least 5% of the total fissile mass. This threshold will not be reached when just a few atoms of ^{233}U are present from the decay chain of ^{237}Np, which is created in small quantities from several sources in a uranium-fueled reactor. If essentially no ^{235}U is present, label 640 ^{233}U Isotopic Content may be used. Only one label from 640 ^{233}U, 660 ^{233}U + ^{235}U, and 670 ^{235}U is used in any given entry. Plutonium isotopics are not typically known, therefore the element is always reported as label 700 Plutonium rather than any of the individual isotope labels, 710-760.

Fixed data elements are given in Table 5.4. Labels 010 Report Type and 309 Entry Status and Cross-Reference Code are fixed for the type of report being generated, a new ICR. If CNTAUR was expanded to also generate the other types of nuclear material accounting reports, PIL and MBR, then 010 Report Type would be expanded to change relative to the report type.

Table 5.2: Data elements calculated from simulated data alone

Label	Name	Description
002	Entry Number / Total Number of Entries	Numbers the specific entry within the set of accounting entry
003	Report Date	The date on which the report was produced
015	Reporting Period	The period covered by the report
412	Date of Inventory Change	Date on which an inventory change occurred
436	Operator's Material Description Text	Unformatted description of the batch in free text
446	Batch Name	Uniquely identifies a portion of nuclear material handled as a unit for accounting purposes

Table 5.3: Weight data implemented

Label	Name	Unit
610	NU	kg
620	DU	kg
630	Enriched uranium	g
640	^{233}U isotopic content	g
660	^{233}U + ^{235}U isotopic content	g
670	^{235}U isotopic content	g
700	Plutonium	g
800	Thorium	kg

Table 5.4: Fixed data elements

Label	Name	Description
010	Report Type	I for Inventory Change Report
309	Entry Status and Cross-Reference Code	N for new entry
469	Measurement Identification Code	N for fixed batch measurement data. Indicates when and where the batch was last measured
470	Number of Items in the Batch	1 item

Table 5.5: Data elements relying on information from the MBA and/or MDC files

Label	Name	Description
001	Reference Number	Uniquely identifies a report for filing, processing, and sorting
006	Encoder's Name	The name of the official responsible for the report
207	Facility Code	Identifies the reporting facility
307	MBA Code	Identifies the reporting material balance area
370	Shipper of Nuclear Material	Identifies the shipper of the nuclear material
372	Receiver of Nuclear Material	Identifies the receiver of the nuclear material
407	Key Measurement Point Code	Incoming or outgoing flow KMP
411	Type of Inventory Change	Defines the type of transaction reported or a material balance item
430	Material Description Code	Four characters describing the physical form, chemical form, volume/ material containment, and irradiation status/quality of the material

Unusual reports and entries, such as correcting a previously-submitted report, or reports for explanation and clarification (Concise Note entries and Textual Reports) are not currently implemented.

Label 469 Measurement Identification Code is the one label fixed due to a gap in current Cyclus capabilities. Cyclus simulations do not have a concept of material measurement, and masses and isotopic fractions are known exactly in a simulation. It is possible to simulate measurements post-hoc in simulation output, which has been demonstrated by Burke *et. al* [36] at PNNL. This capability has not yet been expanded to encompass an entire simulation, or incorporated directly into Cyclus, which would be a more robust solution. Because the information required to vary Label 469 Measurement Identification Code is not available, the value is fixed for all entries.

Many labels are based directly on simulated output but require additional context about the nuclear material accounting structures in a State, such as the MBAs and country codes. These labels are given in Table 5.5. Label 006 Encoder's Name is a command-line input for Cntaur, otherwise a placeholder value is used. Label 430 Material Description Code requires the information from the additional MDC input file described in Section 5.2.3, and the rest of the labels in Table 5.5 require information from the MBA file, also described in Section 5.2.3. All labels not available in the current version of Cntaur are listed in Appendix C.2.1, and are not relevant to the objectives of this project.

Detailed information on each label is available from the IAEA in the Model Subsidiary Arrangement Code 10 Contents, Format and Structure of Reports to the Agency [110].

5.2.2 Development of Cntaur

Cntaur is an analysis tool built on the Cyclus ecosystem. Any fuel cycle that can be modeled with Cyclus can be turned into synthetic labeled-format Code 10 ICRs using only a simulation output database and two additional user-input files, described in Section 5.2.3.

One challenge that has arisen with the use of an agent-based fuel cycle simulator for generating synthetic accountancy is the tracking of process changes to materials within an MBA. Agents using the Cyclus application programming interface (API), which allows third-party nuclear facility models to plug into a simulation, are not required to report their process for making nuclear changes to the material it owns. The standard set of facility models called Cycamore, does record this information, but third-party models that do not participate in the inventory reporting process may detailed ICR tracking.

To develop a tool that is most able to take advantage of the systems already in place, inventory changes that occur from nuclear changes are identified using the transactions that occur between agents in a facility. This is implemented by checking whether a resource has undergone a compositional change since it entered the facility from which it is recorded as leaving. This requires that every structure that triggers a formal inventory change, namely crossing MBA boundaries or permanent discharge of UNF, must be replicated as individual agents in a simulation so that movements between them are recorded on the transactions database.

5.2.3 Cntaur input data

Cntaur takes a Cyclus simulation output file, an MBA file, and an MDC file and generates ICRs for each MBA of interest. Accounting reports can be generated in labeled format, one of the three standard formats that the IAEA will accept. Additionally, the same data can be saved in a convenient CSV format where column headers are the labels and rows are entries in a report.

Three files are needed to run Cntaur and generate synthetic nuclear material accounting reports. The output of a Cyclus simulation, an MBA file, and a MDC file. The bulk of the data needed to run Cntaur is contained within a standard Cyclus output file.

5.2.3.1 MBA file

The MBA file is where the user provides the bridge to connect their simulation agents to the nuclear material accounting structures of MBAs and KMP. This file is also where users note which MBAs the user wants accounting reports to be generated for.

Designating MBAs as areas that don't generate reports can be used to represent other countries. Transactions to or from MBAs or countries designated not to generate reports will result in unmatched transactions, or transactions which are only recorded on one ICR as either the sender or receiver and not the other. These transactions are not truly "unmatched" in the sense that they have no corresponding partner, but simply that the trading partner crosses a State boundary. Therefore, the other transaction is the responsibility of the other State.

Individual agents can also be tagged as ghosts, which will not generate reports, and transactions to or from those locations will not be recorded at all. This technique can be used to clean up parts of the simulation that handle accounting-irrelevant non-nuclear material like the extra fluorine produced after deconversion or to test out nefarious "undeclared" actors.

Individual agents can be tagged as reactors, or as enrichment, which denotes nuclear loss and production or uranium category changes respectively. This ensures that these key inventory changes are captured as report entries even when they occur within the bounds of an MBA, which would otherwise not trigger an inventory change.

An example snippet of an MBA file declaration for a simplified nuclear reactor, represented by a reactor and a spent fuel pool, is given in Appendix C as Listing C.3. Designating a reactor agent, in this case `Reactor_Id15`, ensures that nuclear loss and production are calculated upon final discharge of the fuel.

5.2.3.2 MDC file

A MDC file is also needed because Cyclus currently lacks a flag to designate nuclear material as being contained in the context that the IAEA requires. Nuclear materials in a simulation are also only designated by mass, without any necessary density measurements that could be used to determine the relevant volumes. The current version of Cntaur uses an additional user-input file that links relevant material description code to the Cntaur material description management of commodities, however future updates to Cyclus may be able to automate away the need for an additional MDC file. Appendix C contains an example snippet of a MDC file, linking user-defined commodity names in Cyclus corresponding to a particular type of nuclear material to their physical form, chemical form, containment and irradiation status/quality codes.

Table 5.6 reproduces some of the most commonly used physical form, chemical form, containment, and irradiation status and quality codes. For example, uranium dixode fuel assemblies being shipped from a fuel fabrication plant would be tagged as “B/Q/2/F", because they are complete fuel elements “B”, a dioxide chemical form UO_2 “Q”, in a fresh fuel shipping container regardless if they’re shipped as one or several assemblies “2”, and are non-irradiated fuel elements “F”.

Table 5.6: Commonly used material description codes

(*a*) Commonly used physical form codes

Code	Key word
B	Fuel elements
F	Powders
G	Powder, ceramic
O	Solids, other

(*b*) Commonly used chemical form codes

Code	Key word
D	Elemental
G	Hex
Q	Dioxide
U	Oxide (3/8)
5	Zr alloys

(*c*) Commonly used containment codes

Code	Key word
1	Uncontained
2	Fuel units
3	Flask
Q	Container with volume $\geqslant$200 L and $\leqslant$500 L

(*d*) Commonly used irradiation status and quality codes

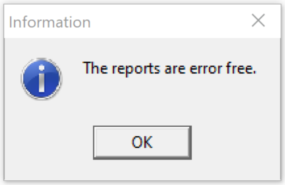
Code	Key word	Irradiated
F	Fuel	N
G	Fuel	Y
B	Pure, stable	N
J	Pure, stable	Y

An example MDC file for the same very simple reactor system as listed above is given in Appendix C as Listing C.4.

5.2.4 Validation

A version of the IAEA-developed software to validate nuclear material accounting reports against the Code 10 style for format compliance, Quality Control Verification Software (QCVS) was acquired [56]. Along with a Code 10 subject matter expert (SME), QCVS was used to ensure that CNTAUR was replicating nuclear material accounting reports correctly. Fictitious countries that do not share country codes with any existing countries were developed to use in all test cases. CNTAUR-created test data, including the simplified single-facility country described above and further detailed in Appendix C, have successfully passed QCVS quality control checks.

(*a*) *IAEA developed Quality Control Verification Software*



The reports are error free.

(*b*) *Quality Control checks verify whether a snippet is compliant*

Only synthetic model fuel cycles are used as demonstrations without any claim to model a real State. The gathering of State-specific information steps mimics realistic gathering of (fictitious) information.

5.3 Summary

This project developed a new capability to reflect nuclear fuel cycle simulations as Code 10-style IAEA nuclear material accounting reports. Coupled with the ability to model diverse and complex nuclear fuel cycles using the Cyclus nuclear fuel cycle simulator, this presents a powerful new tool that can generate large amounts of synthetic data. Any nuclear fuel cycle that can be modeled in Cyclus can be used to generate synthetic nuclear material accounting reports.

This capability can be used as a virtual test bed to accelerate the development of novel data processing techniques to more efficiently and effectively analyze State nuclear material accounting reports. By generating data based on the format and content that States with CSAs submit to the IAEA, data scientists and analysts can focus on leveraging advancements in data processing techniques for safeguards evaluation. Because the tool builds on the Cyclus ecosystem, future developments of nuclear process and facility models for the Cyclus ecosystem can also be used to generate synthetic nuclear material accounting reports for advanced fuel cycles.

6 FICTITIOUS FUEL CYCLES

This work builds on prior work identifying and categorizing types of nuclear fuel cycles [111] and addresses recommendations to develop a set of well-defined case studies that capture the breadth of potential fuel cycles while defining enough detail to actually model a scenario with cradle-to-grave nuclear material movement [52].

These case studies will be particularly useful in demonstrating the functionality developed in Sections 4 and 5. International safeguards is a discipline where politics and perceptions of fairness can be front and center, especially so when developing computational tools designed to mimic or identify potential diversions of nuclear material. There are also limitations and sensitivity concerns from some regular sponsors of international safeguards-related research.

For this reason, scenarios used to demonstrate software developments should not exactly mimic real States. There has been no systematic development of a set of broad-ranging case studies that capture common existing fuel cycles, such as ones based on large LWRs and heavy water reactors (HWRs), while also including advanced fuel cycles.

This capability is required to demonstrate the work described in Sections 4 and 5, but also as a reusable set of test cases for any future nuclear fuel cycle simulation work where State-level demonstrations are required or desired but real countries cannot be used.

Test cases are used to demonstrate the functionality of new software capabilities, but in fuel cycle simulations they are often ad-hoc or designed to replicate an existing State or regional fuel cycle. By developing a set of case studies in a systematic way, future developments in existing tools and new nuclear fuel cycle simulators will have the option to demonstrate their improvements on a standardized set of cases.

This can enable comparisons across computational tools, including tools that may not have been benchmarked against each other before.

6.1 Case development

In 2014, a group of researchers from across the U.S. national laboratory complex published the E&S study [1], which created a taxonomy of nuclear fuel cycles resulting in over 4,000 individual options and reduced them to forty evaluation groups (EG) using parameters listed in Table 6.1. These parameters form the first layer of reactor and fuel cycle discrimination used in this work. The E&S study also defined nine Evaluation Criteria, given in Table 6.2, to assess the EGs for their possible benefits and challenges of implementation.

Table 6.1: E&S study fuel cycle parameters

Nuclear fuel cycle parameters	Options
Type of recycle	Once-through, limited recycle, continuous recycle
Reactivity	Critical, sub-critical
Neutron spectrum	Thermal, fast (includes intermediate)
Incoming feed fuel material	uranium, uranium-thorium, thorium
Recycled elements	uranium-233, plutonium, TRU
Requires enrichment	Yes, no, no* (*needed for startup)

Each of the seven parameters from the E&S study, in Table 6.1, are described in Section 6.2 and in each case. Some are modified or expanded further to encompass their effects on the entire NFC. Additional parameters are introduced because they are required to develop working fuel cycle models, and because they affect the patterns of nuclear material movement that are reflected in nuclear material accounting reports.

Table 6.2: E&S study Evaluation Criteria

Evaluation criteria
Nuclear Waste Management
Proliferation Risk
Nuclear Material Security Risk
Safety
Environmental Impact
Resource Utilization
Development and Deployment Risk
Institutional Issues
Financial Risk and Economics

This work compiles a small, useful set of scenarios, each containing enough description of the full NFC and capabilities for the development of cradle-to-grave simulations and the ability to be recreated using other nuclear fuel cycle simulators.

The E&S study introduced thousands of fuel cycles and successfully narrowed them to several dozen EG. This work is necessarily an exercise in minimalism; it expands on the study's conclusion while adding additional parameters, but it results in only thirteen cases.

The assessment of the EGs from the E&S study is leveraged to determine the cases that are most valuable to capture as full State-sized fuel cycles. Similarly, the type of recycling is used at the first level of categorization for all cases with three options: once-through, limited-recycle, and continuous recycle.

The E&S study summarized their findings by plotting a generalized benefit against a generalized challenge, reproduced in Figure 6.1 with the EGs expanded into cases highlighted in yellow and areas of interest in green. Benefits increase from zero to one, and the challenge is inverted so that the case representing the current U.S. NFC, EG01, is at 1.0 and lower values represent a higher challenge to develop and deploy.

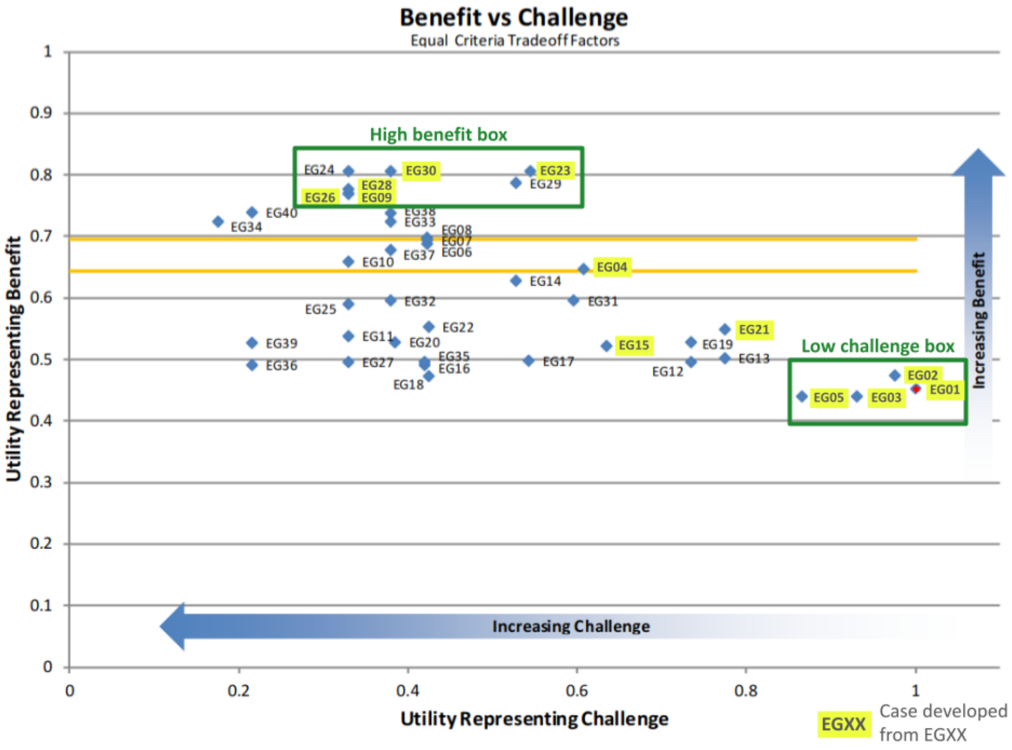


Figure 6.1: Fuel cycle benefit versus normalized challenge for the 40 Evaluation Groups, reproduced from the E&S study [1] with modifications to highlight the EGs selected to become full case studies.

In the bottom right of Figure 6.1 is the low-challenge box containing the EGs with the lowest challenge to implement on a State-wide scale. All of these once-through EGs are included in the case studies. Cases EG01 and EG03 encompass fuel cycles that already exist as LWRs fueled with less than 5% enriched LEU, and HWRs that can be fueled with NU, respectively. EG02 encompasses multiple reactor designs that are in the prototype stage, such as the operating HTR-PM in China, or near-term deployment stage, including several reactors with active demonstration projects in the U.S. like X-energy's Xe-100 [112, 113, 114] and Kairos Power's KP-FHR [115, 116].

EG04 was also added to the group of once-through fuel cycles. Although EG04 has a higher challenge than the other once-through cases, it also has a high benefit per challenge and includes another near-term deployment reactor system, TerraPower's Natrium [117]. The once-through cases are listed in Table 6.3.

For a limited-recycle case, EG09 was selected as the single highest benefit EG of its category, which can be seen in the high-benefit box that is otherwise dominated by continuous recycle cases. While all other selected cases deploy only critical reactors, one EG was selected in order to demonstrate a sub-critical system with an externally-driven system (EDS). Many EGs can or could include EDS, but EG16 was selected to model an existing reactor technology, Pressurized Water Reactors (PWRs), feeding an EDS with the express purpose of burning plutonium. EG16 is the only EG with these parameters that has an actual reactor system available for use in case-building through the Fuel Cycle Options Catalog [118].

For the continuous recycle cases, four of the six EGs in the high-benefit box of Figure 6.1 were selected. EG23, EG24, and EG30 all have the single highest level of benefit. But EG24 is identical to EG23 except for having TRU recycle instead of just recycling plutonium. EG28 was selected instead as being similar but using ^{233}U as well as TRU recycle from uranium-thorium feed fuel and still being a high-benefit case. EG26 is included to model a thorium-feed-only case as well as a case that can be used to model a fluid-fueled Molten Salt Reactor (MSR) with in-line reprocessing.

Finally, EG21 was added to capture nuclear material movement dynamics that were not otherwise included in the other EGs. EG21 can be used to model a two-stage thermal PWR system where all of the recycled/recovered material (RM), in this case plutonium, is recycled into the second stage, and the first stage is only fed by fresh enriched uranium. This case is both relatively plausible considering that it builds on existing reactor designs, and useful for international safeguards because the two stages can be differentiated in their nuclear material accounting reports.

The EGs used as the base of each case are listed in Table 6.3. In the descriptions of each case, Section 6.4, each case notes the EG from which it was derived.

Table 6.3: Evaluation groups selected to become full State-sized case studies

Type of recycle	EG selected to become full cases
Once-through	EG01, EG02, EG03, EG04, EG05
Limited Recycle	EG09, EG15
Continuous Recycle	EG21, EG23, EG26, EG28, EG30

Section 6.2 introduces the scope of features needed to define and create a full working model of each State. First, the features originally used by the E&S study are described, including any changes or modifications made to their original boundaries. Then, several new reactor parameters are introduced that are necessary to turn a reactor system description into a model of nuclear material flow through a NFC, including reactor power, cycle length, and number of batches in-core. Each feature has at least two options, with an example value chosen when a single category covers a range of values, such as high-assay low enriched uranium (HALEU) representing 5% to 20% enriched uranium. Each value of each feature is used in at least one scenario, unless otherwise specified. For simplicity, all States contain either a single reactor type, or only the number of reactor types needed to feed a recycling scheme with multiple stages.

Each case is defined as a set of fuel cycle facilities, with the necessary assumption that any step not located in a State would be available as needed through imports. States are not assigned illogical extraneous facilities, such as an enrichment plant in a country that uses only unenriched fuel. Section 6.3 describes how fuel cycle facilities are developed. Finally, Section 6.4 introduces each case in detail and Section 6.5 provides a summary table for all cases.

6.2 Parameter overview

The primary challenge of creating case studies is determining and prioritizing the features that have a significant impact on the flow of nuclear materials among a long list of variable parameters that define an entire nuclear fuel cycle. The case study parameters, given in Table 6.4, include and expand upon the taxonomy of six parameters defined by the E&S study, which are reproduced in Table 6.1.

Table 6.4: Case study parameters

Type	Parameter
Reactor	Heavy metal composition of fresh fuel
	Uranium-235 enrichment
	Neutron spectrum
	Reactivity
	Reactor power
	Cycle length
	Batches in core
Recycling	Reprocessing
	Recycled elements
	Limited- or continuous recycle
	Stages
Fuel Cycle	Complexity
	Depth
	Total power production
	Facility sizing

None of the parameters are truly independent; they are bound to each other by logic and physics, but some are explicitly dependent on others. For example, uranium-235 enrichment is only relevant for fuel cycles whose fuel mass contains uranium-235, and the material recycled is dependent on whether reprocessing is part of the fuel cycle at all. Each of the features is described in more detail below.

6.2.1 Heavy metal composition of fresh fuel

The composition of heavy metal (HM) in the fuel loaded into nuclear reactors is the central feature in defining the flow of materials throughout an entire nuclear fuel cycle, and is necessarily the first feature used to define a set of comprehensive case studies for fuel cycle simulations. This parameter includes the E&S study parameter "incoming feed fuel material" exactly, as well as the "requires enrichment" parameter with additional enrichment categories.

6.2.1.1 Uranium, including uranium enrichment

Uranium-based fuel is the most common nuclear fuel around the world, and it remains a popular choice among advanced reactor designers for its abundance, comparatively high levels of experience with the nuclear fuel cycle, and existing knowledge of its material properties in common chemical forms like uranium dioxide (UO_2). In the case of modeling pure uranium or mixed-oxide fuel containing uranium, enrichment is the primary method of characterizing uranium in the fuel. Although the E&S report only considers whether enrichment is required for steady-state reactor operation with a flag for enrichment requirements for startup, this project considers five categories of uranium enrichment.

Uranium enrichments for fresh uranium are DU, natural, LEU, HALEU, and HEU as described in Table 6.5. No cases use HEU. Reprocessed uranium (RU) is only available in cases that recycle material, and the enrichment of the material depends on the composition of the UNF. Re-enrichment of RU is not considered. For discussion of uranium-233, see the section on thorium.

This project considers HALEU as a sub-category of LEU to match the IAEA definition of LEU, which considers the upper limit of LEU to be 20% enrichment.

To avoid confusion, enrichments above 5% will be described as HALEU, and only enrichments below 5% but above NU will be described as LEU although they are all technically LEU.

Table 6.5: Representative enrichments by weight percent uranium-235

Name	U-235 w/o% range	Example case
Depleted uranium	[0%, 0.7%)	Case 6
Natural uranium	0.7%	Case 2
Reprocessed uranium	0.5%+[2]	Case 10
Low enriched uranium[1]	(0.72%, 20%)	Case 1
High-assay low enriched uranium	[5%, 20%)	Case 3
Highly enriched uranium	[20%, 100%]	

[1] Some definitions of LEU include only up to 5% enrichment, such that it does not overlap with HALEU and reflects the current NRC restriction on power reactor fuel at 5.0%

[2] Weight percent range based on initial enrichment of fuel

6.2.1.2 Thorium

Thorium, a natural element comprised primarily of the fertile thorium-232 isotope, has been considered as a nuclear fuel throughout the history of nuclear power, although only a handful of reactors have ever used it, mostly at the research and demonstration scale. Thorium-232 is fertile, and requires a neutron source to produce fissile uranium-233. The only way to maintain a purely thorium-fueled nuclear reactor is through an accelerator-driven system or other external source of neutrons (most commonly thorium reactors contain mixed fuels relying on either ^{235}U or plutonium to drive the production of ^{233}U for reactor startup).

Case 13, a MSR with in-line reprocessing of fission products (FP) and transuranics, is the only case using thorium alone as a fresh/makeup fuel.

Table 6.6: Mixed actinide fuels

Actinides	Example case
U-Th	Case 8
U-Pu	Case 9
U-TRU	Case 11
U-Th-Pu/TRU	Case 10

6.2.1.3 Mixed fuels

Uranium is the highest atomic number element present in useful quantities on Earth, although trace amounts of plutonium are present due to neutron capture of ^{238}U from spontaneous fission, as human-created plutonium from nuclear weapons tests, and of cosmic origin. Functionally though, plutonium in quantities needed to fuel a nuclear reactor can only be made by intentionally breeding uranium or by recycling already-created plutonium from used nuclear fuel or nuclear weapons. For this reason, plutonium is unlikely to ever be used as a standalone nuclear material and will always be mixed with uranium and/or thorium, or otherwise derived from a fuel cycle that uses uranium and/or thorium.

The only case that uses pure plutonium fuel is Case 7, which burns pure plutonium fuel from Stage 1 in its EDS Stage 2. Thorium-plutonium/TRU as a mixed fuel is dependent on existing stocks of plutonium or a fuel cycle that also includes uranium-based reactor systems to produce new plutonium, as Th-Pu systems burn much more plutonium than they produce. No thorium-plutonium/TRU cases are included in the case studies.

6.2.1.4 Minor Actinides

Minor actinide (MA) include all the transuranic elements produced in nuclear reactors with the exception of plutonium, although this is frequently simplified to focus only the highest-yield actinides of neptunium, americium, and curium. Protactinium is included for thorium-based fuel cycles. Due to their long half-lives and domination of the activity of UNF in the timeframe beyond hundreds of years, one option is to burn them in a recycle fuel cycle.

At the primary factor level, the recycling of MA is treated as a binary. Either all neptunium, curium, and americium is recovered and placed into the fuel fabrication stream, or none is. This feature is also commonly tied to the use of recycled plutonium in nuclear fuels. The combination of MA and plutonium can be described as TRU material. The presence of MA in fuel cannot be treated as an independent parameter, as it is tied to the material recycled. See the section on reprocessing, 6.2.6 for more detail.

Table 6.7: Presence of Minor Actinides in Closed Fuel Cycles

Name	MA recycled	Example case
Minor Actinide Fuel	Pa, Np, Am, Cm	Case 6
Minor Actinide Disposal	None	Case 10

6.2.2 Neutron Spectrum

Neutron spectra are reported as either fast or thermal as shown in Table 6.8, following the convention of the E&S study. The behavior of intermediate, or epithermal, spectrum systems was deemed similar enough to fast spectrum by the E&S study so as to not warrant their own EGs.

Table 6.8: Neutron spectrum options

Name	Key features	Example case
Thermal	Presence of moderator	Case 1
Fast	Typical conversion ratio of near unity	Case 5

6.2.3 Reactivity

All commercialized nuclear power systems so far have relied on critical systems, which can maintain a self-sustaining nuclear chain reaction. Sub-critical systems, which cannot maintain a chain reaction alone, are used in research and may someday have commercial power applications. Reactivity is one of the core six parameters used in the E&S study and reproduced here, with the two options shown in Table 6.9.

The most commonly proposed sub-critical systems are accelerator-driven system (ADS) or fission-fusion hybrid systems, the latter of which has seen renewed research interest due to the large number of nuclear fusion start-up companies aiming to commercialize fusion in the 2030s. This work does not consider fusion systems, and does not differentiate between the source of external neutrons. Sub-critical systems are generically referred to as EDS.

Table 6.9: Reactivity options

Name	Key features	Example case
Critical	Self-sustaining nuclear chain reaction	Case 1
Sub-critical/EDS	External neutron source required	Case 7

6.2.4 Core mass

The E&S study did not consider reactor size or throughput metrics in its parameter space, because it considered only energy-normalized continuous equilibrium systems. However, the mass and mass throughput of reactors are fundamental aspects of building a NFC simulation for international safeguards analysis. Since the scenario must produce the correct amount of material at the correct time, it is not enough to simply classify throughput by mass per unit time, such as kilograms per year. For example, a reactor that refuels one-seventh of its core annually may have the same average throughput as a reactor that refuels its entire core once every seven years, but they would not result in the same pattern of requests for fresh fuel.

This metric can be defined in a number of ways, including the mass of ore mined per timestep, the mass of standardized un-enriched material such as UOC or UF_6 produced per timestep, or mass of fuel needed per timestep or per reactor cycle, which is most useful in a setting where there is high levels of standardization in reactor types, fuel masses, and cycle lengths.

Each case study focuses on the most limited set of facilities needed to demonstrate the capabilities needed to model certain technologies or facility types. Therefore, the primary metrics used to characterize mass throughput are heavy metal mass in-core, cycle length, and batching information.

Cycle length and batching are often combined into a single metric of average time spent in operation, typically given in units of effective full-power days (EFPD). This parameter is useful in reactor analysis, but is inadequate for fuel cycle modeling which is concerned with the patterns of nuclear material flow. A reactor that refuels its entire core once every 10 years can have the same assembly EFPD as a reactor that refuels annually, with 10 batches. However, the first reactor will only need fresh fuel once a decade, with a large order each time, while the second reactor will need fuel fabricated each year. Therefore, core throughput is disambiguated into cycle length and number of batches.

6.2.4.1 Reactor power

For solid-fueled reactors, fuel is typically housed in assemblies or fuel compacts, each of which has an average or expected mass of fissile and fertile nuclides. For fluid-filled reactors, the relevant masses would include the in-core heavy metal mass, as well as the fuel circuit heavy metal mass. For the base scenarios, fluid-fueled reactors are not considered, nor is fuel that is discharged for one or more cycles and then later returned to the core. When some amount of nuclear material is removed from the core, it is only either returned to operation or permanently discharged.

With this caveat, the mass of fissile and fertile nuclides in-core feature is bounded both by physics and engineering convention. There is a lower bound of nuclear material needed for a reactor; no critical reactor will be smaller than an infinitely reflected critical mass. Practically, the smallest reactors used for commercial production rather than research are still above that mass to produce a usable amount of heat for a sufficiently long time. The upper bound of core mass is set by the largest proposed power reactors.

Nuclear power reactors are typically categorized by their electrical or thermal output rather than the mass of fuel loaded in the core, so this metric is used to classify the size of a reactor. Reactors are sized as micro[1], small[2] , medium [125], and the rest are large reactors. Where an accepted value is given only in megawatts-electric (MWe), an assumption is made that the value is associated with a typical LWR thermal efficiency of approximately one-third and converted to megawatts-thermal accordingly.

Table 6.10: Reactor power options with representative values

Mass description	Thermal Range (MWth)	Example case
Micro	$\leqslant 30$	Case 4
Small	(30, 1000]	Case 3
Medium	(1000, 2100]	Case 8
Large	> 2100	Case 1

6.2.5 Cycle Length and Batching

Cycle length can be defined by the time between reactor refueling outages. Batching refers to the fraction of the core replaced during each outage.

The parameters used for cycle length and batching are core-averaged and given for an equilibrium system. They are therefore a simplification of a system that for some cases is much more complicated. For example, with pebble bed systems the pebbles discharged per EFPD and the rate of pebbles recycled back into the core varies between multiple stages. At the HTR-10 prototype reactor in China, there

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[1] There is no widely accepted cutoff, either in MWth or MWe between micro and small reactors. U.S. Government Accountability Office (GAO) has defined microreactors as "generating less than 50 megawatts electric" [119]. The DOE Gateway for Accelerated Innovation in Nuclear (GAIN) program webpage on DOE microreactors says they "[t]ypically produce less than 20 MWth" [120]. World Nuclear Association (WNA) calls them very small, saying the term is "proposed for units under about 15 MWe" [121]. Where possible, IAEA definitions are accepted, so in this case microreactors is capped at 30 MWth/approximately 10 MWe [122, 123]

[2] The cutoff between small and other reactors, often deemed conventional, is more widely accepted at 300 MWe [124].

Table 6.11: Cycle length options with representative values

Cycle length description	Range	Example value
Online	[<1 day, 1 month)	1 day / Case 2
Short	[1 month day, 1 year)	4 months / Case 6
Medium	[1 year, 5 years)	18 months / Case 5
Long	5+ years	5 years / Case 4

Table 6.12: Effective batches with representative values

Batching description	Range	Example value
Very Low	1	1 / Case 4
Low	[2-10)	3 / Case 1
Medium	[10, 100)	34 / Case 5
High	[100, 250)	190 / Case 2
Very High	250+	1050 / Case 3

are four fuel management stages as described by Yang *et al.* [126]: initial startup, transition from cold to hot full power and no fuel discharge, increasing volume fraction of fuel vs graphite elements, and finally equilibrium system.

Many fuel cycle modeling tools were not designed to simulate online or continuous refueling of reactors. This scenario arises in the case of liquid-fueled reactors, in which fuel is constantly circulating into and out of the core with the coolant, or in the case of solid-fueled reactors such as CANada Deuterium Uranium (CANDU) which push individual assemblies into or out of the core on a more frequent basis than reactors that must shut down to refuel their cores. However, it should be noted that CANDU and other online-refueled reactors still require maintenance outages, and any high-fidelity modeling that captures capacity factors should still reflect average outage lengths and frequencies. In 2021, Canada's Darlington 1 reactor operated continuously for 1106 days, slightly over three years, breaking the record for longest continuously-operating reactor in the world [127].

In the case of online or continuous circulation of fuel, the mass throughput is defined as the rate that new fuel is added to the core/old fuel is permanent retired from the core.

6.2.6 Reprocessing

Reprocessing is the most important parameter in the E&S study because it has the largest impact on several of the study's Evaluation Criteria (Table 6.2) including resource utilization, nuclear waste management, development and deployment risk, and environmental impact. This work uses the same three parameters: type of recycling, stages, and recycled elements.

Nuclear reprocessing chemically separates UNF into N streams based on elements, with N depending on the process used. This can be done in order to recover fissile and/or fertile nuclear material to be used in fabrication of nuclear fuel, which decreases the amount of uranium or thorium needing to enter the fuel cycle through mining. This material might not be reused immediately, but instead stored as potential future fuel for advanced nuclear fuel cycle that isn't yet operating in the State. Reprocessing of material can also be advantageous for the disposal of UNF by separating fission products, which dominate the activity profile in the first hundreds of years after discharge, from the actinides which have much longer half-lives.

Shuffling bundles within a reactor core between cycles or replacing a fuel bundle back into the core after an outage without any physical modification is excluded from the definition of recycling and would still fall under the category of once-through fuel cycles.

While reprocessing is a necessary component of a recycling-based (closed) nuclear fuel cycle, reprocessing could still be used for its disposal properties within a open nuclear fuel cycle.

6.2.6.1 Recycled elements

The simplified components of UNF are described in Table 6.13. While the E&S study only categorized reactor systems by whether they recycled uranium-233, plutonium, and/or TRU, this work also notes where RU (all isotopes) and thorium are recycled, and to which stage each type of RM is reused in.

Table 6.13: Simplified components of used nuclear fuel

Component	Description
Uranium	All isotopes
Thorium	N/A
Plutonium	All isotopes
MA	Neptunium, americium, and curium
FP	All other elements

Reprocessing schemes can be broken up into seven major types as shown in Table 6.14, some of which can be redundant or irrelevant depending on the rest of the fuel cycle present. A once-through fuel cycle may include R&D on reprocessing, as long as there is no commercial-scale separation and recycle of UNF. These types do not represent all possible combinations of the four major recycled elements of used nuclear fuel (excludes FP), rather only the ones that are most reasonable to be implemented in a real fuel cycle. For example, it is unlikely that a fuel cycle would recycle only thorium and MA, leaving behind valuable fissile isotopes of uranium and/or plutonium. There is also a no-recycle option, which was not considered by the E&S study. In the no-recycle option, reprocessing of UNF occurs, separating the material into component streams, but there is no recycling back into reactor fuel.

This option does not reduce the mining needs of a case but can be useful in reducing the mass of long-lived high level waste (HLW) that requires the most robust (and expensive) disposal solution.

Table 6.14: Overview of reprocessing options

Name	Th	U	Pu	MA
Once-through				
No recycle				
U-Th recycle	✓	✓		
U-Pu recycle		✓	✓	
Pu recycle			✓	
TRU recycle			✓	✓
All recycle	✓	✓	✓	✓

Regardless of reprocessing option, the material that is being reused rather than stored or disposed of can be collectively called RM, to distinguish it from fresh uranium or thorium. RU is a subcategory of RM that refers to uranium alone.

More complex reprocessing schemes, such as direct use of spent PWR fuel in CANDU (DUPIC) cycles that siphon gaseous fission products but leave the solid discharged fuel as-is[128], recycling of americium alone[129], and (re)enrichment of RU to produce more desirable isotopics are not considered.

Reprocessing without recycling

Reprocessing may be undertaken with the goal of reducing the volumetric capacity of a future permanent disposal solution for HLW. The number and elemental makeup of each reprocessing product may vary, but one proposed policy could result in products and outcomes as described in Table 6.15.

Table 6.15: Potential disposition pathways for fuel cycle employing reprocessing without recycling

Stream	Outcome
Transuranics	Deep geologic disposal
Uranium	Shallow disposal
Thorium	Shallow disposal
Fission products	Surface storage on the order of hundreds of years

6.2.7 Limited-recycle or continuous recycle

Limited recycle, twice-through

Most recycling of nuclear material to-date has not been a true closed nuclear fuel cycle, but rather semi-closed. In this case, UNF is recycled and some nuclides, typically uranium and/or plutonium, are recycled into new nuclear fuel, but are then discharged and disposed of after the second round.

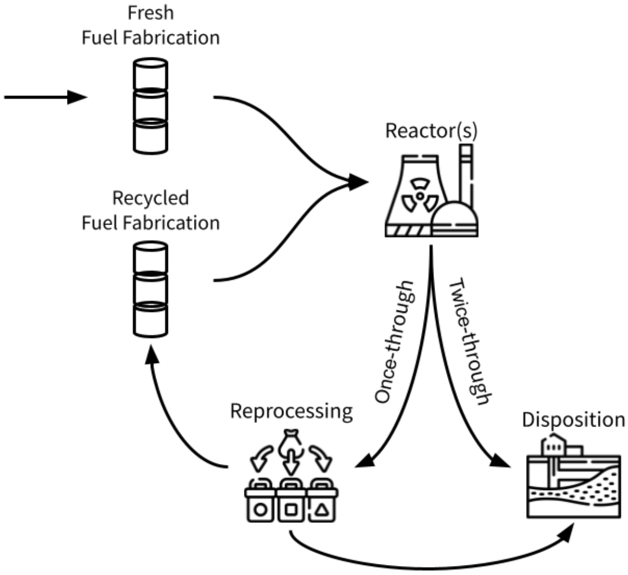

Figure 6.2: Monorecycling with a single stage. Fresh fuel is used in one or more reactors, the used fuel is separated and re-made into mixed-actinide fuel, and then returned to the same set of reactors before final disposition. Multirecycle would have all material returning to the reprocessing step regardless of how many times it has been through the reactor.

Continuous recycle

Continuous recycling can produce the most efficient use of mined resources, assuming the availability of all necessary reprocessing and reactor technologies to do so. In this case, UNF is recycled into new fuel, re-burned, and recycled again ad infinitum.

6.2.8 Use of stages

Recycling, both limited- and continuous recycle, can be described as either single-stage or multi-stage.

One-stage recycling, depicted in Figure 6.2 with a mono-recycle strategy, typically relies on a single design of set of reactors. Since the availability of recycled fuel will always be strictly less than the fuel needed for the next cycle, one-stage recycling either fuels reactors with a limited number of recycled assemblies along with raw ones, or only feeds recycled assemblies into a core every n cycles.

Multi-stage recycling segregates reactors as either fueled with only raw fuel or fueled with some or all recycled material. A depiction is given in Figure 6.3. This can present in several different ways, such as an identical fleet of reactors, a small fraction reserved from the rest as being fueled with recycled material, or a fleet of one reactor style burning material for use in another. One such example is a fleet of thermal water reactors burning raw material for a single fast-spectrum breeder reactor.

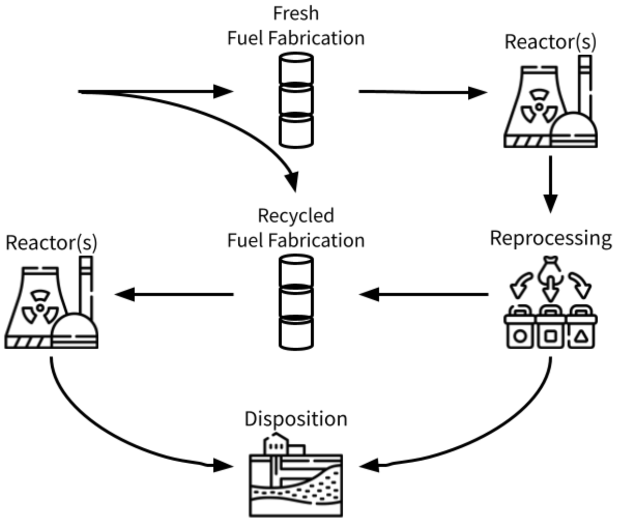

Figure 6.3: Monorecycling with two stages. The first set of reactors is only fueled with fresh fuel, and the recycled fuel is used in a separate set of reactors

6.2.9 Depth and complexity of fuel cycle

For a State to have a fully self-sufficient and independent nuclear fuel cycle, it must have a variety of technical capabilities and facilities that range from resource extraction, to fuel manufacturing, to reactor design and construction, to waste management.

In reality, most nuclear fuel cycles are integrated into a global market. This often presents as a lack of available economic uranium and/or thorium reserves or a lack of interest/economic drivers/technical know-how to engage with complicated processes such as uranium enrichment, reactor design, or reprocessing. Similarly, countries without nuclear power reactors may still have enough uranium and thorium reserves to prompt recovery and export.

Table 6.16 describes the simplified facilities and processes considered for the depth and complexity of each case study.

The above facilities and processes can be mixed and matched in many ways. Each of the above facilities has a minimum complexity, as shown in Table 6.17.

Table 6.16: Types of fuel cycle facilities that could be deployed in a case

Type	Description
Front end	Uranium mining, conventional and *in-situ* leaching (ISL), and milling Thorium mining and milling Conversion Enrichment Fresh fuel fabrication including de-conversion where applicable
Back end	Reprocessing Recycled fuel fabrication Consolidated interim waste storage
Other	Research reactors R&D on hot cells and/or reprocessing R&D on uranium enrichment Other R&D facilities with special nuclear material (SNM) Heavy water production

The depth and complexity of a fuel cycle would be determined by the highest complexity level facility present. For example, a State with only commercial reactors and mining/milling activities would be categorized as low, while a State with the aforementioned facilities plus reprocessing would be classified as high complexity.

Table 6.17: Minimum complexity associated with the presence of nuclear fuel cycle facilities or activities

Min level	Fuel cycle facilities
Low	Mine and milling, conversion, consolidated long-term waste storage or disposal, research reactors, other R&D activities containing SNM
Medium	Fresh fuel fabrication, R&D hot cells/reprocessing, R&D enrichment, heavy water production
High	Enrichment, reprocessing, recycled fuel fabrication

Importantly, the fuel cycle complexity metric does not determine the capability to build additional facilities. For example, a low-complexity State may have the capacity to fabricate fuel but not currently have a domestic facility. Having research facilities on enrichment technologies, reprocessing, or other R&D activities concerning the nuclear fuel cycle may indicate a State's capability to move up in the complexity scale within the near future, but this is not explicitly modeled or considered.

Depth of the nuclear fuel cycle is a secondary metric intended to recognize that the number of fuel cycle facilities in a State is separate from the technical complexity of those facilities. Table 6.18 shows the cutoff between the two levels, shallow and deep.

Table 6.18: Depth associated with the number of types of fuel cycle facilities & activities present in a State

Depth	Categories of fuel cycle facilities & activities
Shallow	Three or fewer[1]
Deep	Four or more

[1] Facilities not counting towards number of activities: other R&D activities

A medium-complexity State may have a "complete" fuel cycle, in that no external nuclear services are required for their fuel cycle, while a high-complexity State may only have one fuel cycle facility, such as enrichment. Table 6.19 gives examples of permutations for each of the three complexity and two depth parameters.

Depth and complexity are both related to the number of fuel cycle facilities that exist in a State rather than the services required, which may required exports and imports from another State. Use of enrichment and/or reprocessing services from another State does not place a State at high complexity; only the facilities within a State count toward the complexity designation.

Table 6.19: Examples of depth and complexity permutations

Complexity	Depth	Example
Low	Shallow	Mine/milling
	Deep	Mine/milling, conversion, consolidated long-term waste storage or disposal, research reactors
Medium	Shallow	Mine/milling, R&D hot cells
	Deep	Fuel fabrication, consolidated storage or disposal, research reactors, SNM R&D activities
High	Shallow	Enrichment, consolidated long-term waste storage or disposal, SNM R&D activities
	Deep	Mine/milling, conversion, enrichment, fresh fuel fabrication, reprocessing, recycled fuel fabrication research reactors, R&D enrichment, hot cells, and other activities containing SNM

6.2.10 Total power production

All reactors are assumed to be producing exclusively electricity using their thermal power. Cases are assigned a total power production level across their whole fleets, from four categories listed in Table 6.20. Reactors are deployed to collectively produce approximately their given power level.

Total power production is correlated to reactor mass, and only logical combinations are assigned to cases. For example, a case with microreactors of 5 MWe should not be assigned a system-wide 100 GWe of production, which would require the deployment of 20,000 reactors. Similarly, large reactors are not deployed at the 1 or 0.1 GWe levels to allow at least two reactors to be deployed per case with the exception of Case 13, where there is a single fluid-fueled MSR with online reprocessing.

Table 6.20: Total power production

Description	Power value
Very Low	0.1 GWe
Low	1 GWe
Medium	10 GWe
High	100 GWe

6.3 Facility details

All fuel cycle facilities are developed in a standardized manner. Model fuel cycle facilities are developed below with several standard sizes, which are deployed directly into cases. Each fuel cycle facility (reactor) deployed from a model fuel cycle facility (reactor) system is functionally identical.

6.3.0.1 Power Reactors

For all cases, a single reactor reactor design is deployed for one-stage systems or up to two reactor designs for multi-stage systems (one design for each stage). Model reactors represent existing reactors, reactor designs that have applied for reactor licenses, reactor systems that have been included in the DOE Fuel Cycle Options Catalog[130, 118], or other reactor designs with significant publication histories by U.S. national laboratories, in decreasing order of preference. No new reactor systems were designed for this project. Cases that use reactor systems from the Fuel Cycle Options Catalog will be referenced primarily by their option title.

Reactor systems are characterized as one of the following general types: LWRs which includes both PWRs and Boiling Water Reactors (BWRs), HWRs, High Temperature Gas-Cooled Reactor (HTGR), Sodium-Cooled Fast Reactors (SFRs), MSRs, heat pipe reactors, and EDSs which makes no distinction between fission-fusion hybrid systems, ADS, or other sources of external neutrons. These are not a comprehensive set of all reactor systems that can be designed, but they represent a wide scope of reactor designs and the cases could be modified as-needed to swap out reactors, such as replacing a SFR with a Lead-Cooled Fast Reactor (LFR).

For reactors with regular refueling that is correlated to the calendar year, cycle start dates were sampled randomly from a uniform distribution within two annual date blocks, spring, and fall. The cycles roughly correspond to March 1st to May 15th for spring, and September 1st to November 15th for fall. Unless resource constraints prevent enough fresh fuel from being available, plants have perfectly periodic cycles. An example, 4-unit LWR plant with an 18-month refueling cycle could have the following first cycle described in Table 6.21.

Reactor	Cycle start	Calendar date	Outage start	Calendar date
1	123	May 3rd, 2025	650	October 12th, 2026
2	301	November 9th, 2025	840	April 20th, 2027
3	452	March 28th, 2026	979	Sept. 6th, 2027
4	622	Sept. 14th, 2026	1149	February 23rd

Table 6.21: Example reactor cycles for a multi-unit plant with single-day time steps

All simulations are designed with a start-up period in order to reach steady state as quickly as possible. The start-up period is from the first simulation day (January 1st, 2025) until the last reactor has fueled and begun its cycle. The `Cycamore:Reactor` model requires that reactors obtain a full core worth of material to begin operating; they do not start with a partial-core as if they have had previous operational cycles pre-simulation. In order to achieve the designed cycles as described above, additional fresh fuel is available only during the run-up to cycle start for each reactor to help them start on time. This is achieved with additional agents that create fuel and additional fresh fuel vault agents that can stage material to fuel the reactor. These agents are also important because they provide the initial cores of reactors that have separate initial fuel and equilibrium fuel materials or enrichments. No transition period is modeled in these cases– they are assumed to be fueled with their equilibrium batches starting after the first cycle. The agents that provide full-core startup fuel are retired after the start-up period and the simulation proceeds at equilibrium.

Cases with either very short or long cycle lengths have reactor start dates sampled randomly from the calendar year. Reactors that refuel more frequently than once a year are assumed to purchase fuel approximately once a year.

Power plant facilities are composed of one or more reactors. Each reactor is deployed with its own fresh fuel vault agent. UNF pools may be shared among multiple reactors. Each power plant has only one agent that packages UNF into transport canisters and ships the material to CIS facilities, where applicable.

The only exceptions to the above model are individual microreactor facilities that are refueled as a full-core replacement. These facilities do not have any on-site UNF storage or shipment facilities; they are directly moved to the back-end CIS facility.

6.3.0.2 Fuel Cycle Front End

Following the same assumptions made by the 2013 U.S. DOE Fuel Cycle Options Campaign Evaluation & Screening report[111], no losses are modeled for mining/milling, conversion to uranium hexafluoride (UF_6) for enrichment, conversion to metal, oxide, or other fuel form for unenriched fuels, enrichment, and deconversion of UF_6.

Uranium fuel cycles start with UOC, either domestically produced or imported. The material is modeled as 100% uranium oxide (U_3O_8). No differentiation is made between ISL mining and milled materials from open-pit or underground mining. Thorium fuel cycles begin with refined thorium as thorium dixoide (ThO_2). If the reactor system uses thorium oxide, no additional conversion is included, otherwise the thorium is converted to the the chemical form of the fresh fuel in a conversion plant[131].

Uranium enrichment is modeled as a SWU-based system. All tails are 0.25%, regardless of product enrichment. Fuel fabrication losses are modeled as 0.2%. All fuel fabrication facilities are assumed to have identical capacities for deconversion, pelletizing, and rod/assembly/compact forming, where applicable.

Fuel cycle facilities have standard sizing across all cases. For each type of facility in a given case, one of five standard size options are deployed. Sizes were developed based on existing worldwide fuel cycle facilities, with the smallest and largest standard facility options set at approximately 30% above or below real-world facilities. Figure 6.22 describes the standard sizing in the most generic units applicable. When deployed as Cyclus agents in a simulation, these sizing parameters are converted into the relevant throughput units such as tUO_2/time step. When thorium and uranium fuels are used in a system, facility throughput is split between processing the two elements as applicable to the fuel form.

Table 6.22: Standard fuel cycle facility sizes

Facility	X-Small	Small	Medium	Large	X-Large
Mining/milling (tHM/year)	1,000	4,000	7,500	15,000	30,000
Conversion (tU/year)	5,000	7,500	12,500	15,000	20,000
Enrichment (tSWU/year)	1,000	3,000	5,000	10,000	12,500
Fresh fuel fabrication (tHM/year)	100	250	750	1,500	2,500

6.3.0.3 Fuel Cycle Back End and Other R&D

Reprocessing losses are modeled as 1.0%, following the convention of the E&S study. Reprocessing, and multi-actinide fuel fabrications are the exception to the standard sizing model described in Section 6.3.0.2. Because reprocessing is used very sparingly in current fuel cycles, and not all reprocessing strategies are present in existing recycling facilities, fuel cycle facility sizes for reprocessing and mixed-actinide fuel fabrication were not created based solely on existing facilities as front-end facilities are. Instead, facilities are always sized to meet the throughput needed for the reactor systems that use the RM. There is no under-sizing or over-sizing with import.

CIS are sized based on 50 years of that case's UNF production. In some cases, the capacity may be split between several equally sized facilities. There is no under-sizing or over-sizing. The fuel cycle ends with CIS facilities, which can replicate surface-level dry storage, wet storage pools, or even underground repositories with recoverable fuel. No differentiation is made between the type of CIS facility.

Research reactors assigned to cases from one of three standard types. The training type is modeled after the General Atomics TRIGA reactor deployed in multiple countries[132, **?**], the research reactor is modeled after the LVR-15 research reactor in the Czech Republic[133, 134], and the low-power reactor is modeled after the Walthousen Reactor Critical Facility at Rensselaer Polytechnic Institute in the United States[135]. The reactor parameters are given in Table 6.23. Cases can have more than one type of research reactor, and multiple reactors of each type can be deployed, up to three per type.

Other key R&D facilities are modeled as possessing or processing small amounts of nuclear material. Most R&D facilities do not interface with the commercial fuel

Table 6.23: Research reactor types and parameters

Type	Power	Assembly size	In core	Effective batches	Cycle time	Refuel time
Training	1 MW	2.25 kg	57	57	729 days	1 days
Research	10 MW	1.71 kg	28	7	28 days	14 days
Low-power	100 W	0.832 kg	333	1	100 years	1 days

cycle, except a hot cell/reprocessing R&D facility which may transact a small amount of UNF into the facility.

6.3.0.4 Nuclear material packaging and transportation

Using the new capabilities designed to model nuclear material packages and transport units described in Chapter 4, cases may package nuclear materials at every step in the fuel cycle. Where applicable, existing package types are used, such as a 24-assembly multi-purpose canister (MPC) for PWR fuel. A few examples of packaging are given in Table 6.24. Additional packaging and transport details are in Appendix C.1.

Table 6.24: Example nuclear material packages

Nuclear material	Package	Fill max (kg)
UOC/ThO_2	210 L/55 gal drums	350
Natural UF_6	Type 48Y cylinders	12,501
$\leqslant$5% UF_6	Type 30B cylinders	2277
LWR assemblies	Westinghouse 17x17	615.2
TRISO pebbles	Versa-Pac VP-55 (400 pebbles)	2.8

6.4 Case descriptions

Case development prioritized several objectives. Cases are logical and plausible. Reactor systems are linked to an EG from the E&S study using Table 6.3. Reactors are developed directly from public information released by reactor design companies, from cases in the Fuel Cycle Options database [136], or paper reactors in literature with enough information to build a fuel cycle simulation around them.

Once-through cases prioritize reactor systems that currently exist or could plausibly exist in the forthcoming decades either by development of a nuclear newcomer nation or as a subset of nuclear facilities in a country with an existing fuel cycle. For example, a country with existing medium/large thermal LWRs could build out a case 5 system on top of or as a replacement for its existing fuel cycle.

Enrichment is likely to play a larger role for countries that have once-through systems, so these case studies are more carefully designed to include systems that require LEU or HALEU, which many reactor design companies rely on. Recycle case studies prioritized fuel cycle systems derived more directly from EGs in the DOE E&S study [1].

6.4.1 Case 1

Case 1 is based on large thermal LWRs with LEU fuel and no recycling. The fuel form is UO_2 assemblies. This case is most similar to many current fuel cycles. The reactor system is modeled on the American Westinghouse AP1000 PWR [137]. This case matches the characteristics of EG01, the reference case from the E&S study.

Figure 6.4 is the nuclear fuel cycle diagram for this case, with three import points and three export points. For this and all such diagrams, research facilities including research reactors are not included.

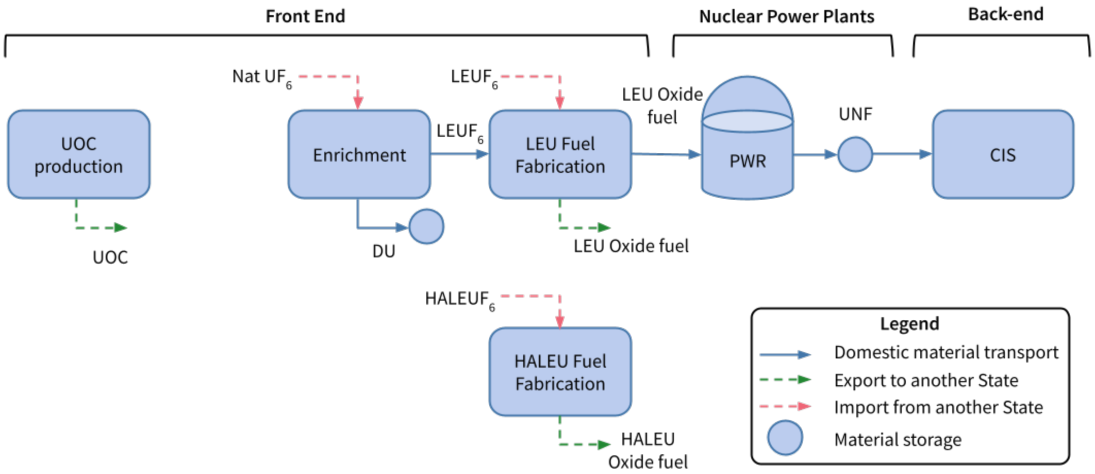

Figure 6.4: Case 1 simplified facility and nuclear material flow diagram

The case parameter overview is given in Table 6.25. To support the 10 GWe system, a total of ten operational reactors are deployed. The startup period is two years, at which point all reactors are operational.

Power plants in case 1 are built in four-packs, with two UNF pools per plant. As this case is similar to existing large nuclear nations, many of which have been operating long enough to shut down reactors, six decommissioned reactors across two power plants are also included. One power plant includes two decommissioned and two operating reactors.

The list of fuel cycle facilities in the case are given in Table 6.26. This case produces a significant amount of UOC, all exported. Because the case has undersized enrichment capacity, additional make-up enriched UF_6 must be imported into the LEU fuel fabrication stage. The fuel fabrication facility is oversized, so excess capacity beyond the case's requirements is exported. The facility also has a HALEU production line, which does not fuel any of the power plants and is instead exported.

Table 6.25: Case 1 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium	
	Enrichment	LEU	4.8% initial, 4.5% equilibrium
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Medium	18 months
	Effective batches	Low	3
	EG	EG01	
Reprocessing	Once-through		
Fuel Cycle	Complexity	High	Enrichment
	Depth	Deep	Five facility types
	Total power	Medium	10 GWe, 10 reactors

Table 6.26: Case 1 fuel cycle

Facility	Size
UOC production	Large
Enrichment	Small
Fuel Fabrication	Medium
CIS	1 Facility
Decommissioned	6 reactors
Other R&D	Yes

Research reactor	Number
Training	2
Medical	1
Zero-power	0

6.4.2 Case 2

Case 2 is based on medium-sized, thermal HWRs with NU fuel and no recycling. The fuel form is UO_2 bundles. The reactor system is modeled on the Canadian AtkinsRéalis (formerly SNC-Lavalin) CANDU 6 reactor [138]. This case matches the characteristics of EG03. Figure 6.5 shows the case facility overview.

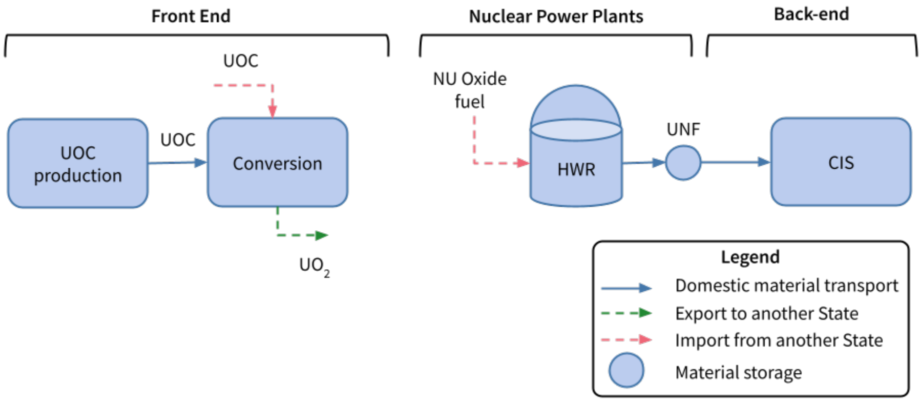

Figure 6.5: Case 2 simplified facility and nuclear material flow diagram

The reactor system is given in Table 6.27. Reactors produce 600 MWe each. This case is at the 100 GWe total power level, so 167 operating reactors are deployed. Refueling operations are conducted daily. Because the basic reactor model used in these case studies (`Cycamore:Reactor`) does not separate refueling from other outages, these reactors do not undergo non-refueling maintenance outages as similar real systems do.

The mass throughput was estimated by spatially-averaging the channel dwell times across the core. For a reference CANDU 6 reactor, the dwell times range from 158 EFPD to 356, with an average EFPD of 192 [139].

Some of the features distinguishing Case 2 from Case 1include high-frequency discharges of UNF, resulting in daily accounting records of nuclear loss and production, and NU fresh fuel.

The startup period is one year, with all reactors starting on a randomly selected date in the first year. Power plants have eight reactors, and each reactor has its own UNF wet storage.

This case has a very small UOC production facility and a large conversion plant that imports additional UOC and produces both UO_2 for domestic consumption

Table 6.27: Case 2 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium	
	Enrichment	NU	0.7%
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Medium	600 MWe
	Cycle length	Online	1 day
	Effective batches	High	190
	EG	EG03	
Reprocessing	Once-through		
Fuel Cycle	Complexity	Low	
	Depth	Deep	4 facility types
	Total power	High	100 GWe, 167 reactors

and export as well as UF_6 for export.

There is one fully decommissioned power plant with eight reactors. There is one medical and one zero-power research reactor.

Table 6.28: Case 2 fuel cycle

Facility	Size
UOC production	X-Small
Conversion	Large
CIS	2 Facilities
Decommissioned	8 reactors
Heavy water	Yes

Research reactor	Number
Training	0
Medical	1
Zero-power	1

6.4.3 Case 3

Case 3 is built around HALEU thermal small modular reactor (SMR) designs. The reactor system is an HTGR that does not use recycling. The reference reactor system is the HTR-PM pebble bed reactor in Shandong Province, China [140, 141]. The fuel form is Tristructural Isotropic (TRISO) fuel pebbles with 8.5% enriched uranium. This case matches the characteristics of EG02.

Figure 6.6 shows the case facilities, with the reactor parameters given in Table 6.31 and the fuel cycle system described in Table 6.32.

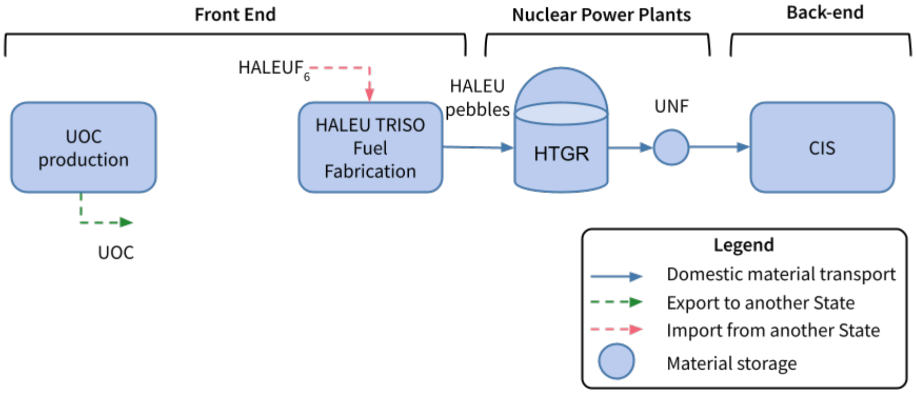

Figure 6.6: Case 3 simplified facility and nuclear material flow diagram

While pebble bed reactors continuously cycle pebbles, refueling in this case is modeled as occurring once per time step, *i.e.* once per day. Fuel items are also modeled as one batch, or approximately 400 TRISO pebbles due to the large number of fuel elements in a pebble-bed reactor. Because the basic reactor model used in these case studies, `Cycamore:Reactor`, does not separate out refueling outages from other outages, these reactors do not undergo non-refueling maintenance outages as similar real systems do.

This case is differentiated from previous cases by having HALEU fuel. Although modeling this reactor using the `Cycamore:Reactor` archetype would result in exactly

400 pebbles being discharged daily, a higher-fidelity reactor model could also capture that the average daily discharge mass might be represented more effectively by a bulk quantized packaged material that varies from day-to-day.

Table 6.29: Case 3 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium	
	Enrichment	HALEU	8.5%
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Small	105 MWe
	Cycle length	Online	Continuous
	Effective batches	Very High	1050
	EG	EG02	
Reprocessing	Once-through		
Fuel Cycle	Complexity	Medium	
	Depth	Deep	Four facility types
	Total power	Medium	10 GWe, 95 reactors

This case has UOC production and fuel fabrication. There are five decommissioned reactors in addition to the 95 operating reactors. There is only one research reactor, a training reactor.

The fuel cycle complexity of this case is medium, because of the fuel facility but also because the state has an active R&D program on enrichment and hopes to develop a domestic enrichment capability in the upcoming years.

Table 6.30: Case 3 fuel cycle

Facility	Size
UOC production	Small
Fuel fabrication	Small
CIS	1 Facility
Decommissioned	5 reactors
R&D enrichment	Yes

Research reactor	Number
Training	1
Medical	0
Zero-power	0

6.4.4 Case 4

Case 4 includes a fast microreactor heat-pipe system using HALEU fuel. The fuel is UO_2. The fuel cycle does not reprocess. The reference is the Mega-Power reactor designed by McClure *et. al* at LANL, sometimes called the Special Purpose Reactor (SPR), with the Design A core modifications proposed by Sterbentz *et. al* at Idaho National Laboratory (INL) [142, 143]. This case is also most similar to the characteristics of EG02, like 6.4.3, although this case has key differences in neutron spectrum, power, cycle length, and batching, as well as fuel cycle factors. The simplified flow diagram is shown in Figure 6.7.

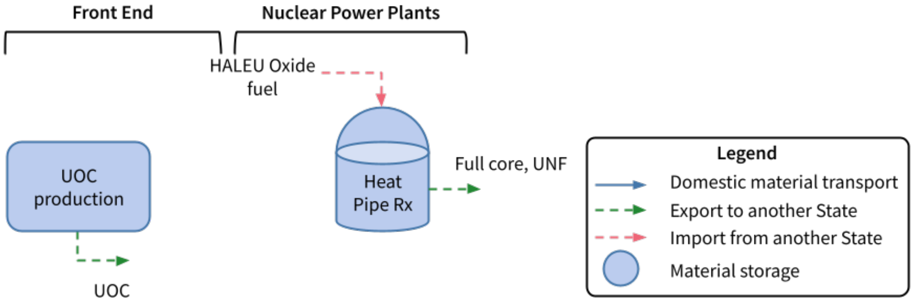

Figure 6.7: Case 4 simplified facility and nuclear material flow diagram

This is the simplest case. This case represents a country that has no real nuclear industry except for large enough uranium resources to have a thriving uranium mining and milling industry. There are no other fuel cycle facilities to speak of, including research reactors. This is also the only case to feature a complete reactor take-back system, where the full core is replaced at the end of the cycle and the entire UNF is exported out of the country, leading to only one batch of fuel per core. The rest of the reactor parameters are given in Table 6.31.

Case 4 has the simplest set of nuclear material movements of any case. Reactors have only one batch, with the full core, including the fuel load, being moved at the end of a cycle.

The fuel cycle is given in Table 6.32. This case represents an ultra-low complexity fuel cycle, in that the only relevant expertise needed by the country could be its regulatory authority and health physicists in the mining industry for UOC production. The nation providing the nuclear power plants could reasonably supply almost all of the other technical capabilities needed to run the system, including plant operation. There is one zero-power reactor.

Table 6.31: Case 4 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium	
	Enrichment	HALEU	19.75%
	Neutron spectrum	Fast	
	Reactivity	Critical	
	Power	Micro	2 MWe
	Cycle length	Long	5 years
	Effective batches	Very Low	1
	EG	EG02	
Reprocessing	Once-through		
Fuel Cycle	Complexity	Low	
	Depth	Shallow	1 facility type
	Total power	Very Low	0.1 GWe, 50 reactors

This case could also be a subset of a larger country. Because microreactors are likely used for special purposes like off-grid production in remote or island communities [144], the entirety of this case could be combined with another case to represent a more complex system, such as a nation with typical small to large reactors for grid scale production and a separate case 4 fleet of microreactors for entirely independent uses.

Similarly, the base development of these case studies represents systems reaching a steady state, so this case was not necessarily designed to represent disaster relief or other fluid situations where reactors may be transported, set up, and run for a period of time less than one cycle length before being removed. But this case could be modified to represent such a circumstance due to the use of mobile cores with long cycle lengths and very small power outputs.

Table 6.32: Case 4 fuel cycle

Facility	Size
UOC production	Medium

Research reactor	Number
Training	0
Medical	0
Zero-power	1

6.4.5 Case 5

Case 5 is a large SFR designed as a breed-and-burn (B&B) system with cycle lengths similar to large LWRs but a large number of batches (34). This is the final no-recycling case study. The reference design is the ANL-created Sustainable Sodium-Cooled Fast Reactor (SSFR) [145, 146] with metallic uranium-zirconium alloy fuel. The reactors are initially loaded with uranium fuel enriched at several levels, all within the category of HALEU. The initial fuel load is modeled with the average

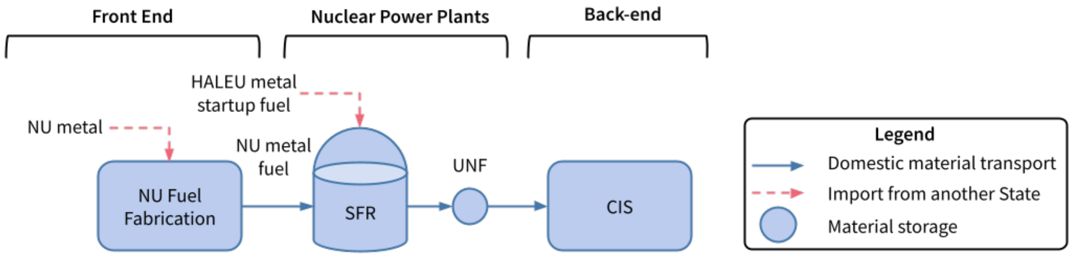

Figure 6.8: Case 5 simplified facility and nuclear material flow diagram

start-up enrichment level of 10.1%. Reactor reloading is completed with NU fuel as enough plutonium is bred into the system. This case matches the characteristics of EG04, which has the highest level of benefit for a once-through system. The flow diagram is given in Figure 6.8.

The reactor in this case is a B&B reactor designed with long fuel lifetimes to breed plutonium into the fuel but also use up much of the plutonium before the fuel is discharged and disposed of. A B&B reactor system can have relatively high resource utilization without the need for reprocessing of UNF. The fuel dwell times in this case are over 50 years (>18,000 EFPD), an order of magnitude longer than most other cases' reactor systems. The case parameters are given in Table 6.33.

Power plants have two reactors per plant and one UNF cooling pool. There are no decommissioned reactors or any research reactors in the state.

Table 6.34 describes the fuel cycle in Case 5. There is only a small fuel fabrication plant in the country, but it is still large enough to satisfy the domestic demand, in part because only a relatively small fraction of the fuel mass is replaced each cycle. There is active research requiring the use of hot cells, which has a single UNF assembly that is being used to research reprocessing technologies.

Table 6.33: Case 5 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium	
	Enrichment	HALEU	10.1% average initial
		NU	0.7% equilibrium
	Neutron spectrum	Fast	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Medium	1.5 years
	Effective batches	Medium	34
	EG	EG04	
Reprocessing	Once-through		
Fuel Cycle	Complexity	Medium	Fuel fabrication R&D hot cells/reprocessing
	Depth	Shallow	3 facility types
	Total power	Low	1 GWe, 10 reactors

Table 6.34: Case 5 fuel cycle

Facility	Size
Fuel fabrication	XS
CIS	2 Facilities
R&D hot cells/ reprocessing	Yes

Research reactor	Number
Training	0
Medical	0
Zero-power	0

6.4.6 Case 6

Case 6 is the first of the three limited recycle cases. The system is a large, one-stage SFR with an equilibrium refueling core of DU. The fuel form is metallic fuel pins modeled as a simplified U-Zr binary and U-TRU-Zr ternary alloy. All RM, which includes RU and TRU, is recycled back into the first stage after melt-refining. Figure 6.9 contains the case overview diagram.

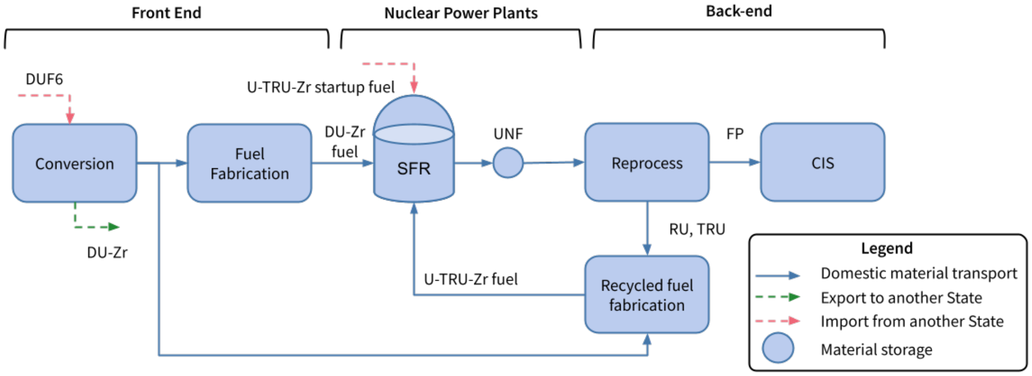

Figure 6.9: Case 6 simplified facility and nuclear material flow diagram

The reactor described in Table 6.35 matches EG09. This EG is listed in the second group of "*Potentially Promising Fuel Cycle*[*s*]" in the E&S study. Similar to EG04 used in Case 5, EG09 is the highest benefit EG in its category of limited-recycle, and is the only group not using continuous recycle to be in the top category of benefit. The system is derived from Fuel Cycle Options catalog "Sodium-Cooled Fast Reactor (Breed and Burn) using Natural Uranium Fuel with limited recycling". The reference reactor in this system was designed by Florent Heidet at the University of California, Berkeley [147], which itself was scaled up to a 3000 MWth/1000 MWe system from the 1000 MWth Advanced Burner Reactor (ABR) designed at ANL [148].

These reactors could be started with an initial core using HALEU fuel or by using an existing stockpile of TRU material to make mixed-actinide fuel. In this case, it is assumed that TRU is available from reprocessed UNF from a now-decommissioned fleet of LWRs each with a lifetime of 50 years.

This case, along with Case 5 and Case 9 are intended to demonstrate similar reactor systems, all using one-stage SFRs, across the three different recycling systems. This case has limited recycle of TRU, while Case 5 does not recycle and Case 9 has continuous recycle of Pu.

While the core contains eight effective batches, half of the core (or four batches)

Table 6.35: Case 6 parameters

Type	Name	Category	Detail
Reactor (Stage 1)	HM in fuel	Uranium initial driver, blanket TRU equilibrium	
	Enrichment	DU	0.25% equilibrium
	Neutron spectrum	Fast	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Long	8.8 years
	Effective batches	Low	8
	EG	EG09	
Reprocess	Recycle type	Limited-recycle	
	Strategy	TRU, RU	
	Material recycled	All RM to Stage 1	
	Stages	1 Stage	
	Number of recycles	Mono/Limited	
Fuel Cycle	Complexity	High	Reprocessing, Recycled fuel fabrication
	Depth	Deep	Four facility types
	Total power	Medium	10 GWe, 10 reactors

are modified at the end of each cycle. One batch is permanently discharged, and three more undergo melt-refining to remove some of the FPs without actinide separation.

The melt-refining process removes most of the gaseous, volatile, and reactive FPs, leaving behind noble and seminoble FPs and some actinides. There is no separation of actinides into individual streams. Uranium, neptunium, and plutonium remain but thorium and americium are removed at 95%+ efficiency [149]. After melt-refining the batch returns to the core for additional cycles before discharge. Fresh fuel batches contain DU-Zr fuel from the fresh fuel fabrication plant.

Table 6.36: Case 6 fuel cycle

Facility	Size
Conversion to DU metal	M
Fresh fuel fabrication	XS
Reprocessing	Yes
Recycled fuel fabrication	Yes
CIS	1 facility
Decommissioned	25 reactors

Research reactor	Number
Training	2
Medical	2
Zero-power	0

The fuel cycle is listed in Table 6.36. Domestic facilities include conversion from DU in UF_6 to U-Zr, some of which is used for fresh fuel fabrication and makeup fuel after melt-refining, with the rest exported. The case has domestic reprocessing capabilities and refabrication plants, which receive the bulk RU and TRU (minus thorium and americium) from the reprocessing plant for re-use as metallic driver fuel.

The case is at the 10 GWe level, which requires 10 SFR. Because melt-refining occurs on three-eights of the core at the end of each cycle, the reprocessing and recycled fuel fabrication capabilities are assumed to be co-located with the plants. Six reactors are co-located with one set of back-end facilities, and the other four reactors are co-located with a second. A single CIS facility is used to store the waste from reprocessing as well as the permanently-discharged fuel. There are also two training and two medical-type research reactors.

A related Fuel Cycle Data Package (FCDP) system from the Fuel Cycle Options Catalog [118], “PWR(LEU) to SFR(Pu/RU) for limited recycling" provides the basis for estimating the Pu and MA available from a now-decommissioned PWR fleet for use as the initial core of the SFRs. Assuming a fixed 50-year lifetime for UNF generation, this case is assigned 25 decommissioned LWRs. UNF is assumed to be already separated into TRU for re-use, and RU and FP which is stored at the CIS facility.

6.4.7 Case 7

Case 7 is the only limited-recycle case study to use a two-stage system. The reactor in the first stage is a large PWR, using the Westinghouse AP1000 as the reference design, the same as Case 1. The second stage is a small subcritical EDS fueled exclusively with the plutonium recovered from Stage 1. The EDS system was modified from the PRISM reactor design by Yang and Khalil to be a subcritical transuranic-burning system [150]. Figure 6.10 gives the case flow diagram.

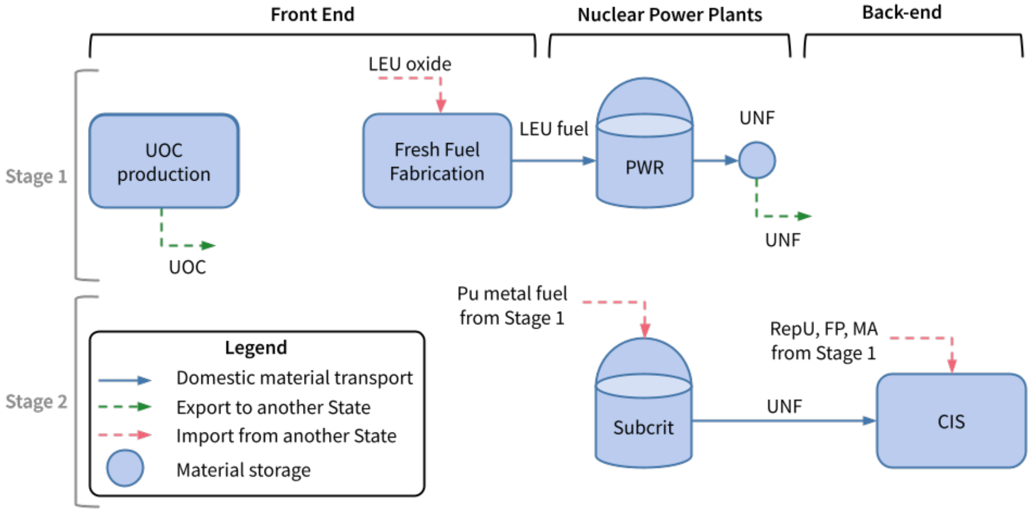

Figure 6.10: Case 7 simplified facility and nuclear material flow diagram

The reactors and basic fuel cycle parameters match EG15, and the system is derived from Fuel Cycle Options catalog system "Pressurized Water Reactor using Low-Enriched Uranium Fuel; Accelerator Driven System using Plutonium Fuel". Each of the two reactor designs are described in the reactor overview in Table 6.37.

Case 7 is the only case that has a stage of reactors fueled with no uranium or thorium. From a nuclear material accounting perspective, the subcritical Stage 2 fuel loads will only be accounted for using the plutonium elemental entry.

Table 6.37: Case 7 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium	
(Stage 1)	Enrichment	LEU	4.5% average
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Medium	18 months
	Effective batches	Low	3
Reactor	HM in fuel	Plutonium	
(Stage 2)	Enrichment	N/A	
	Neutron spectrum	Fast	
	Reactivity	EDS	
	Power	Small	311 MWe
	Cycle length	Very short	9 months
	Effective batches	Low	3
	EG	EG15	
Reprocess	Recycle type	Limited-recycle	
	Strategy	Pu	
	Material recycled	Pu to Stage 2	
	Stages	2 Stages	
	Number of recycles	Single	
Fuel Cycle	Complexity	Medium	Fuel fabrication
	Depth	Shallow	2 facility types
	Total power	High	100 GWe
		92 reactors Stage 1	
		24 reactors Stage 1	

EG16 is used as the base for this case to demonstrate the use of enrichment at the equilibrium stage in a limited-recycle case study. The smilar Evaluation Group

EG14, identical except for not needing enrichment, was listed in the second group of "*Potentially Promising Fuel Cycle*[*s*]".

Table 6.38 gives the case fuel cycle. There are very large facilities for UOC production and fresh fuel fabrication for Stage 1 only. There is no reprocessing or recycled fuel fabrication, so the cooled UNF from the Stage 1 PWRs are exported to another country for both separation and recycled fuel fabrication. The separated RU, MA, and FP are each re-imported and stored in a CIS facility. A separate CIS facility holds the stored UNF fuel after discharge and cooling from the EDSs.

Table 6.38: Case 7 fuel cycle

Facility	Size
UOC production	XL
Fuel fabrication	XL
CIS	2 Facilities

Research reactor	Number
Training	1
Medical	3
Zero-power	0

This case is intended to represent a country that places a high priority on plutonium reduction, perhaps for nonproliferation or other related reasons. However, this case does not have reprocessing or recycled fuel fabrication capability, so UNF from Stage 1 is exported to another State for separation. Plutonium metal fuel is re-imported for use in Stage 2. The rest of the separated material from Stage 1 is also re-imported. The FPs and MA are separated from RU for long-term storage.

6.4.8 Case 8

Case 8 is the final limited-recycling case, and the only one to employ the no-recycle strategy. This represents a country without a current interest in having recycled fuel, but which prioritizes HLW minimization, perhaps to limit the size and complexity of a future disposal facility. A State with this fuel cycle could focus on designing and siting a deep geologic repository (DGR) facility for their long-lived TRU materials, a much smaller mass than the entire UNF. Although this case is listed in the limited-recycle cases because its UNF does get reprocessed and separated into multiple waste streams, this case most closely matches the characteristics of once-through EG05 because the E&S study did not consider reprocessing without recycling, implemented here.

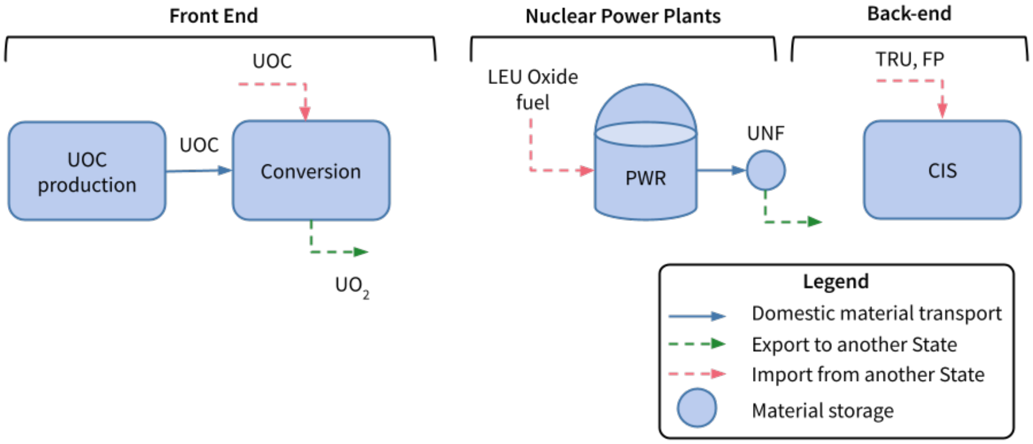

Figure 6.11: Case 8 simplified facility and nuclear material flow diagram

The reactor system is a Westinghouse-style PWR fueled with HALEU and thorium fuel designed by Galperin *et. al* [151]. The system overview is shown in Figure 6.11, and the reactor system is described in Table 6.39.

Similar to Case 7, this case does not have domestic reprocessing facilities. They rely on a supplier State to separate their UNF into thorium, RU, TRU, and FP. The thorium and uranium streams remain in the supplier State, and the other two categories are imported and stored separately for eventual disposal.

This case is the only one that uses both fresh uranium and thorium as makeup fuel. It is also the only one that imports and maintains stockpiles of separated UNF components without current plans for re-use of any of them.

Table 6.39: Case 8 parameters

Type	Name	Category	Detail
Reactor	HM in fuel	Uranium/Thorium	
	Enrichment	HALEU	19.9%
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1130 MWe
	Cycle length	Medium	18 months
	Effective batches		3
Reprocess	Recycle type	Limited-recycle	
	Strategy	TRU, RU	
	Material recycled	N/A	
	Stages	1 Stage	
	Number of recycles	N/A	
Fuel Cycle	Complexity	Low	
	Depth	Shallow	2 facility types
	Total power	Medium	10 GWe
		9 reactors Stage 1	

The domestic fuel cycle in this case is relatively small and is described in Table 6.40: only UOC production and a CIS facility to store the TRU and FP separated by a foreign partner. There are two research reactors, one training and one zero-power.

Table 6.40: Case 8 fuel cycle

Facility	Size
UOC production	M
CIS	1 Facility

Research reactor	Number
Training	1
Medical	0
Zero-power	1

6.4.9 Case 9

Case 9 is the first of the continuous recycle cases, with a single stage of SFRs needing only NU makeup fuel. This case represents the EG with the highest benefit with the lowest challenge from the Evaluation & Screening report, EG23. The challenge level is kept lower by recycling only RU and plutonium and discarding the MA build-up. Figure 6.12 gives a simplified overview of this case.

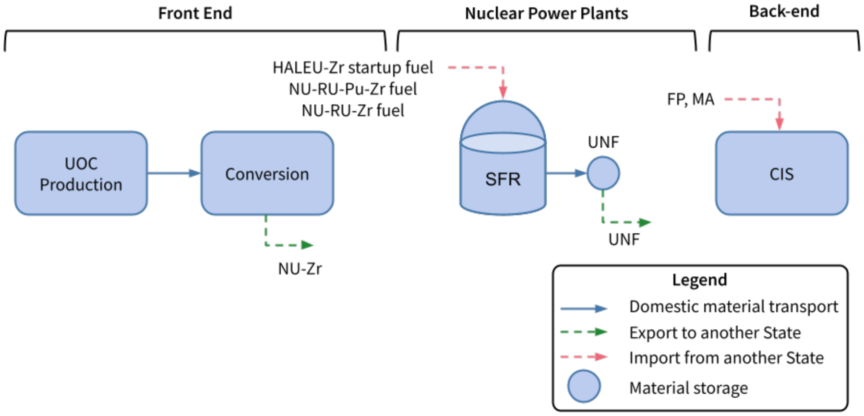

Figure 6.12: Case 9 simplified facility and nuclear material flow diagram

The reactor system was derived from the Fuel Cycle Options Catalog entry “Sodium-Cooled Fast Reactor using Plutonium, Natural Uranium, and Recovered Uranium Fuel”. The reference reactor in this system is the 1000 MWth/380 MWe ABR reference plant designed at ANL [148]. This is the original version of the reactor system that was scaled up to 1000 MWe in Case 5. The fuel is U-Zr metal in the blanket and U-Pu-Zr metal in the driver region. HALEU is used as startup fuel, with recycled fuel used as equilibrium fuel when available.

The case relies on a supplier nation to separate their UNF and fabricate mixed-actinide fuel. Unlike Case 6, which has reprocessing and recycled fuel fabrication facilities co-located with reactors, this case stores UNF in wet storage on site for 5 years before exporting to the supplier nation with reprocessing capabilities.

Table 6.41: Case 9 parameters

Type	Name	Category	Detail
Reactor (Stage 1)	HM in fresh fuel	Uranium	
	Enrichment	HALEU NU	10.1% average initial
	Neutron spectrum	Fast	
	Reactivity	Critical	
	Power	Small	380 MWe
	Cycle length	Short	7 months
	Effective batches	Low	8
	EG	EG23	
Reprocess	Recycle type	Continuous recycle	
	Strategy	Pu, RU	
	Material recycled	All RM to Stage 1	
	Stages	1 Stage	
	Number of recycles	Continuous	
Fuel Cycle	Complexity	Medium	R&D hot cells
	Depth	Deep	4 facility types
	Total power	Medium	10 GWe 26 reactors

However, the country does have an active R&D program with hot cells to research reprocessing techniques, making the fuel complexity medium rather than low.

Table 6.42 contains information about this case's fuel cycle. There are large uranium reserves and a domestic conversion plant that produces both U-Zr and UO_2 for export, including to the country that produces the recycled fuel for their SFRs. Separated FPs and MA are re-imported along with the U-Pu-Zr metal fuel, and they are stored at the country's single CIS facility.

There are four total research reactors, two training-style reactors and two zero-power style reactors. There are no decommissioned reactors.

Table 6.42: Case 9 fuel cycle

Facility	Size
UOC production	L
Conversion	XL
CIS	1 facility
R&D hot cells	2 facilities

Research reactor	Number
Training	2
Medical	0
Zero-power	2

6.4.10 Case 10

Case 10 uses large BWRs using recycled and NU fuel. It is developed based on another high benefit EG, EG28. The primary difference between this EG and EG23 is the recycling of all TRU and ^{233}U, which is produced due to the presence of thorium fertile fuel. It is a continuous recycle case with one stage of fast reactors using thorium and NU oxide fuel in the blanket and recycled RU and plutonium metal fuel in the driver. Both the blanket and driver are reprocessed. The fuel cycle overview diagram is given in Figure 6.13

The model reactor is based on the Resource-renewable Boiling Water Reactor

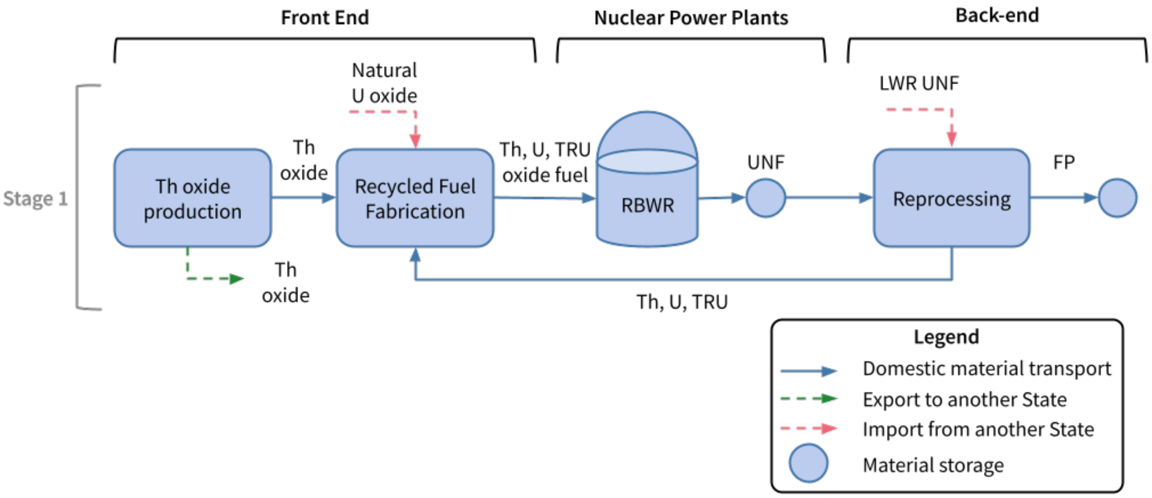

Figure 6.13: Case 10 simplified facility and nuclear material flow diagram

(RBWR) by Hitachi and Hitachi-GE Nuclear Energy [152]. Several configurations of the RBWR have been proposed to burn actinides in a multi-recycle fuel cycle, including the RBWR-AC which maintains a relatively flat actinide concentration, and the RBWR-TB which was designed to burn transuranics from LWR effectively as part of a nuclear exit strategy. A team at Electric Power Research Institute (EPRI) proposed the RBWR-TB2 [153], which can be used in conjunction with a standard LWR fleet to prevent the total TRU population from rising, but before a TRU-burndown with RBWR-TBs.

Table 6.43: Case 10 parameters

Type	Name	Category	Detail
Reactor	HM in fresh fuel	Uranium-thorium	
	Enrichment	NU	
	Neutron spectrum	Intermediate	
	Reactivity	Critical	
	Power	Large	1356 MWe
	Cycle length	Short	337 days
	Effective batches	Low	4.5
	EG	EG23	
Reprocess	Recycle type	Continuous recycle	
	Strategy	Th, ^{233}U/RU, Pu, MA	
	Material recycled	All RM to Stage 1	
	Stages	1 Stage	
	Number of recycles	Continuous	
Fuel Cycle	Complexity	High	Reprocessing
	Depth	Deep	Four facility types
	Total power	Medium	10 GWe 8 reactors

This case uses a version of the RBWR-AC with additional design modifications such that only thorium and NU makeup fuel is required. The exact parameters used are similar but not identical to the RBWR-Th-mixed option designed by Phillip Gorman while at the University of California-Berkeley [154, 155] and is described in Fuel Cycle Options Catalog option "Reduced-Moderation Boiling Water Intermediate Reactor Recycling Transuranics". The case maintains a relatively flat TRU profile through continuous recycles. The reactor system is summarized in Table 6.43.

For a State with domestic thorium reserves and affordable access to significant quantities of NU from another State's current or former enrichment program, this fuel cycle offers high resource utilization and access to domestic makeup fuel. The RBWR technology is more similar to existing LWR technology than some of the other reactor designs used in cases here, especially the SFR and MSR cases.

The RBWR system was originally designed to burn recycled fuel downstream of other reactors, such as typical LWR UNF, or from another configuration of the RBWR system. The reactors in this case are initially fueled with mixed-actinide oxide fuels rather than having a start-up period fueled with enriched uranium. It is assumed that the initial fuel loading is obtained from another State for simplicity, but a version where an older generation of LWRs feeds this design is also possible. Such a system, designed for traditional LWR burning rather than the continuous recycling of a single stage of RBWRs, would be better repressed by another RBWR configuration such as the RBWR-TB [156].

Table 6.44: Case 10 fuel cycle

Facility	Size
ThO_2 production	XS
CIS	1 Facility

Research reactor	Number
Training	1
Medical	1
Zero-power	0

Table 6.44 describes the Case 10 fuel cycle. There are domestic thorium reserves

that are mined, but this country does not have or produce uranium. NU oxide powder is imported to the single fuel fabrication facility, which incorporates fresh and recycled material into multi-zone oxide fuel bundles.

There are two plants with four reactors and one pool for UNF each. UNF is cooled for three years before being sent to the reprocessing facility. This case recycles its own UNF, producing RU, thorium, plutonium, and MA streams that are sent back to the fuel fabrication facility for recycling. FPs are sent to CIS after reprocessing. There is one training and one medical research reactor.

6.4.11 Case 11

Case 11 is a two-stage continuous recycle system that recycles all UNF from Stage 1 of SFRs and Stage 2 of PWRs. The reactor system is derived from the Fuel Cycle Options Catalog entry "Sodium-Cooled Fast Reactor using Transuranic and Uranium Fuel; Pressurized Water Reactor using Transuranic and Uranium Fuel". Figure 6.14 is the case overview diagram.

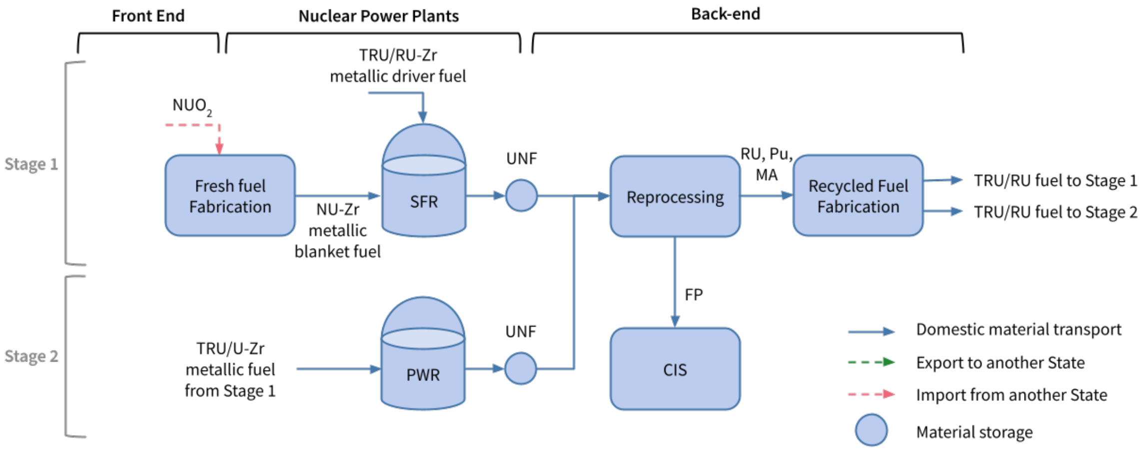

Figure 6.14: Case 11 simplified facility and nuclear material flow diagram

Table 6.45 describes the reactor systems used in this case. Stage 1 is an SFR modeled after the 1000 MWe version of the 380 MWe/1000 MWth ABR designed at ANL [148], as in Case 6 . The driver is fueled with metallic uranium fuel enriched at the HALEU level for the initial core and once-recycled NU-RU-TRU metallic fuel for the equilibrium core. The blanket is comprised of NU and RU metallic fuel. Instead of using existing or imported TRU stockpiles for the initial core like Case 6does with the same design, this case uses HALEU fuel at several enrichments, with an average first-core enrichment level of 10.8%.

Stage 2 is a PWR modeled after the Westinghouse AP1000, same as Case 1and Case 7 [137]. The fuel form is MOX assemblies containing RU and TRU as well as NU.

This case corresponds to EG30, which is one of the highest overall benefit groups, along with EG23 (Case 9 and EG24. EG30 includes both fast and thermal spectrum reactors, while the other two EGs have only fast reactors.

Case 11 has the most complicated recycling scheme of any case. The reactor overview in Table 6.45 briefly describes the flow of material, and Table 6.46 gives a detailed breakdown of recycled material elements by their source. The Stage 1 driver, Stage 1 blanket, and Stage 2 material must all be reprocessed in independent production lines to avoid intermixing of materials designed for reuse in different places. This would result in additional MBAs required in the reprocessing facility, or multiple facilities. All TRU from the Stage 1 driver is recycled to the Stage 1 driver, along with all of the MA from Stage 2 and some TRU from the Stage 1 blanket. The rest of the TRU from the Stage 1 blanket is recycled to Stage 2. The Stage 2 plutonium and RU is all recycled back to Stage 2. RU from the Stage 1 driver is split between the two zones of Stage 2, and the RU from the Stage 1 blanket is split between all three fuel categories as needed. All FPs are sent to the CIS facility for long-term storage.

Table 6.45: Case 11 parameters

Type	Name	Category	Detail
Reactor (Stage 1)	HM in fuel	Uranium initial driver, blanket TRU equilibrium	
	Enrichment	HALEU NU	10.8% average initial
	Neutron spectrum	Fast	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Long	8.8 years
	Effective batches	Low	8
Reactor (Stage 2)	HM in fresh fuel	NU	
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Medium	18 months
	Effective batches	Low	3
	EG	EG30	
Reprocess	Recycle type	Continuous recycle	
	Strategy	TRU, RU	
	Material recycled	Stage 1 Blanket TRU, RU to Stage 1 Stage 1 Driver TRU, RU to Stage 2 Stage 2 MA to Stage 1 Stage 2 Pu, RU to Stage 2	
	Stages	2 Stage	
	Number of recycles	Continuous	
Fuel Cycle	Complexity	High	Reprocessing
	Depth	High	4 facility types
	Total power	High 60 reactors Stage 1 40 reactors Stage 2	100 GWe

Because the UNF components from the blanket and driver of Stage 1 and the fuel of Stage 2 have separate uses in recycled fuel, the reprocessing capabilities must be split into three process lines. One process line each is devoted to the Stage 1 driver fuel, Stage 1 blanket fuel, and Stage 2 fuel, which raises the logistical complexity needed to implement this fuel cycle. Some materials from different sources are combined in the recycled fuel fabrication process, such as the Stage 1 driver combining RU and TRU from the blanket and driver of Stage 1 with the MA from Stage 2, and the blanket of Stage 1 also containing RU from both zones of Stage 1.

Table 6.46: Case 11 has an optimized, but complicated, process for separating and reusing fuel components between the two stages.

Stage	Source (from)	Flow	To Stage 1 Driver	To Stage 1 Blanket	To Stage 2 Driver	To CIS
1	Driver	RU	✓	✓		
		Pu	✓			
		MA	✓			
		FP				✓
	Blanket	RU	✓	✓	✓	
		Pu	✓		✓	
		MA	✓		✓	
		FP				✓
2	Driver	RU			✓	
		Pu			✓	
		MA	✓			
		FP				✓

Table 6.47 gives the fuel cycle overview. This case reprocesses and refabricates its own UNF. Except for the initial cores which contain HALEU metal fuel instead of mixed-actinides, all fuel used in both stages are recycled, so there is no need for domestic fresh fuel fabrication. This case has five research reactors, one of the training style, and two each of the medical and zero-power style.

Table 6.47: Case 11 fuel cycle

Facility	Size
Reprocessing	
Recycled fuel fabrication	
CIS	2 facilities

Research reactor	Number
Training	1
Medical	2
Zero-power	2

6.4.12 Case 12

Case 12 is the only continuous recycle case that relies exclusively on reactor technology that is commonly in commercial use around the world, with two stages of a single PWRs design.

The reactor systems are based on the Fuel Cycle Options Catalog entry "Pressurized Water Reactor using Low-Enriched Uranium Fuel; Pressurized Water Reactor using Plutonium and Recovered Uranium Fuel." The simplified flow diagram is given in Figure 6.15.

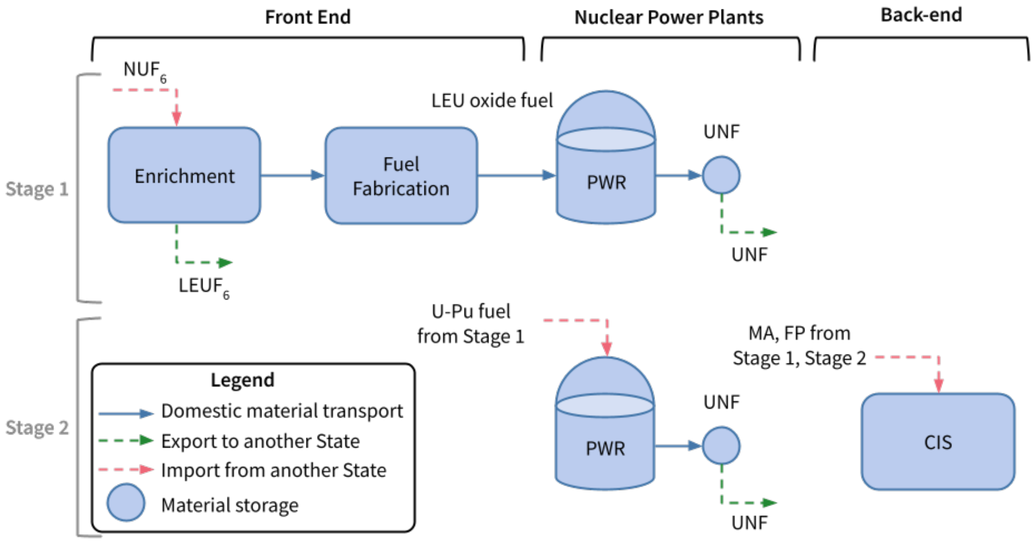

Figure 6.15: Case 12 simplified facility and nuclear material flow diagram

Both reactor systems are Westinghouse AP1000-style PWRs. The fuel form is oxide fuel assemblies, LEU oxide for Stage 1 and both NU oxide and NU-RU-Pu oxide assemblies in Stage 2.

Table 6.48: Case 12 parameters

Type	Name	Category	Detail
Reactor (Stage 1)	HM in fresh fuel	Uranium	
	Enrichment	LEU	
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Medium	18 months
	Effective batches	Low	3
Reactor (Stage 2)	HM in fresh fuel	N/A (only RM)	
	Enrichment	N/A	
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Medium	18 months
	Effective batches	Low	3
	EG	EG21	
Reprocess	Recycle type	Continuous recycle	
	Strategy	RU, Pu	
	Material recycled	All RM to Stage 2	
	Stages	2 Stage	
	Number of recycles	Continuous	
Fuel Cycle	Complexity	High	Enrichment
	Depth	Shallow	Three facility types
	Total power	Medium	10 GWe, 10 reactors 9 reactors Stage 1 1 reactor Stage 2

The recycling strategy of this case is the opposite of Case 11, where material flows back and forth between the two stages after reprocessing. Here, all of the RM from both stages of fuel goes to the second stage for reuse.

The downside of segregating all RM to the second stage of reactors is that the first stage of PWRs requires enrichment. This is the only case that requires both enrichment and the ability to multi-recycle UNF. However, only enrichment capabilities are available domestically; reprocessing services are obtained from a foreign source. Table 6.49 gives the fuel cycle overview for this case. The fresh fuel fabrication plant produces all the fuel for Stage 1 as well as the NU fuel for Stage 2. Two separate product lines in separate MBAs are used to handle the enriched and natural materials.

There are four decommissioned reactors of the same PWR design as Stage 1 and 2 systems. There are three training-style research reactors.

Table 6.49: Case 12 fuel cycle

Facility	Size
Enrichment	L
Fresh fuel fabrication	L
CIS	1 facility
Decommissioned	4 reactors
R&D hot cells	

Research reactor	Number
Training	3
Medical	0
Zero-power	0

6.4.13 Case 13

The final case is a single stage MSR with online reprocessing of TRU in the fuel salt, integrated directly into the reactor. The reactor system used is the ORNL-designed Molten Salt Breeder Reactor (MSBR) [157] as part of an EG26 fuel cycle, with flows defined using the Fuel Cycle Options Catalog "Molten Salt Reactor using Thorium, Uranium-233, and Transuranic Fuel". Case 13 is the only case using a fluid-fueled reactor, and where FPs are separated from actinides in the same facility as the reactor.

Detailed modeling of fuel salt flow through the molten salt separation and treatment systems is outside the scope of this work. The cycle length is the time for the entire fuel salt inventory to undergo chemical separation processing, in this case 10 days. An average thorium makeup rate is used, approximately 2.5 kg per day, which is modeled as 25 kg per cycle.

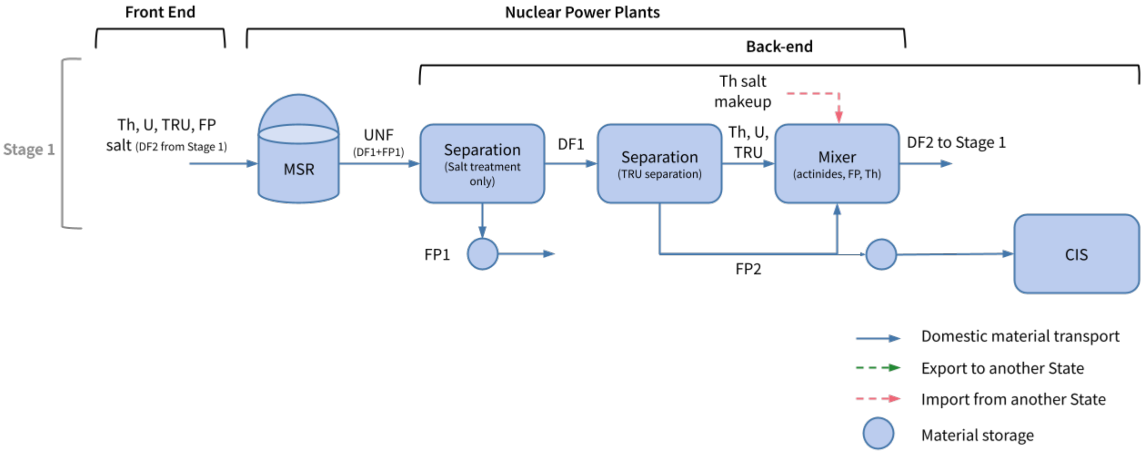

Figure 6.16: Case 13 simplified facility and nuclear material flow diagram

Figure 6.16 gives the fuel cycle system overview. Note that unlike any other recycling case, the fuel separation and reconstitution process is directly integrated into the reactor system, preventing a clean differentiation between the nuclear reactor and the back end of the fuel cycle that is possible in other cases. Two separate FP discharges flow from the reactor. The first is from the off-gas system containing gases, primarily Xe and Kr, noble metals, and solid daughters of the gases [157, 158]. The other FPs stream is from the chemical separation (reprocessing) of the fuel salt, which constantly replaces small amounts of FP and actinide losses with makeup fertile thorium fuel.

A fluid-fueled system with online removal of FPs, especially modeled in an idealized manner, makes such effective use of its nuclear materials that very little

Table 6.50: Case 13 parameters

Type	Name	Category	Detail
Reactor	HM in fresh fuel	Thorium	
	Enrichment	N/A	
	Neutron spectrum	Thermal	
	Reactivity	Critical	
	Power	Large	1000 MWe
	Cycle length	Online	10 days
	Effective batches	Very High	>500
	EG	EG26	
Reprocess	Recycle type	Continuous recycle	
	Strategy	Th, U, Pu, MA, FP	
	Material recycled	All RM to Stage 1	
	Stages	1 Stage	
	Number of recycles	Continuous	
Fuel Cycle	Complexity	High	Reprocessing
	Depth	Shallow	2 Facilities
	Total power	Medium	1 GWe
		1 reactors Stage 1	

makeup thorium fuel salt is necessary.

Table 6.51: Case 13 fuel cycle

Facility	Size
Thorium production	XS
ThF_4 conversion	XS
Reprocessing	

Research reactor	Number
Training	2
Medical	1
Zero-power	0

6.5 Case summary

The cases described above are by no means a comprehensive list of possible fuel cycles. They are a snapshot in time; after the start-up period, they are intended to represent a steady-state system. They also make simplifying assumptions, such as assigning identical facility parameters to reactors of the same style and setting a fixed refueling outage length.

However, the set of cases encompass a wide breadth of parameters describing the reactor systems, recycling processes, and associated required fuel cycle processes that comprise a nuclear fuel cycle.

These cases may be used for demonstrating features, such as in Chapter 7 or benchmarking between nuclear fuel cycle simulation tool across a wide variety of reactor systems. They may also be modified to study system dynamics, such as commissioning or retiring a new reactor or fuel cycle facility, or to study a transition from an existing fuel cycle to one of the cases.

Table 6.52 summarizes some of the key parameters of the cases, including their associated EG and Option Group using the parlance of the E&S study.

Table 6.52: *Case studies with their Evaluation Groups and option details*

#	EG	Recycling	Stage 1			Stage 2			Option Groups[1]
			Reactor	Fuel	RM	Reactor	fuel	RM	
1	EG01	None	PWR	LEU	None				OT-C-T-U-Y
2	EG03	None	HWR	NU	None				OT-C-T-U-N
3	EG02	None	HTGR	HALEU	None				OT-C-T-U-Y
4	EG02	None	Heat pipe	HALEU	None				OT-C-F-U-Y
5	EG04	None	SFR	NU	None				OT-C-F-U-N*
6	EG09	Limited	SFR	DU	RU/TRU				SL-C-F-U-TRU-N*
7	EG15	Limited	PWR	LEU		EDS	None	Pu	ML-C/S-T/F-U-Y
8	EG05	Limited	PWR	HALEU/Th	None				SL-C-T-UTh-Y
9	EG23	Continuous	PWR	NU	RU/Pu				SC-C-T-U-Pu-N*
10	EG24	Continuous	BWR	DU/Th	Th/RU/TRU				SC-C-F-U-TRU-N
11	EG30	Continuous	SFR	NU	RU/TRU	PWR	NU	RU/Pu	MC-C-F/T-U-TRU-N*
12	EG21	Continuous	PWR	LEU	None	PWR	NU	RU/Pu	MC-C-T/T-U-Pu-Y
13	EG26	Continuous	MSR	Th	Th/RU/TRU				SC-C-T-Th-U3/TRU-N*

[1] Option Groups from Appendix B of the E&S study [159] in the style of recycle type - reactivity - neutron spectrum - fresh fuel material - recycled element(s) - enrichment requirements.

7 DEMONSTRATION

The new capabilities described in Chapters 4 and 5 allow Cyclus users to develop more realistic nuclear material movement patterns, inject disruptions into their fuel cycles, and evaluate the impact on the system in the exact format that NNWSs with CSAs submit monthly to the IAEA. The fictitious State cases developed in Chapter 6 show how the new capabilities added to Cyclus and the greater Cyclus ecosystem can affect a country-sized system.

Six of the fictitious cases were developed into full Cyclus simulations and are used throughout this chapter. Table 7.1 also summarizes the key features of each of the six cases chosen.

Table 7.1: Cases used for demonstrations

Case	Recycle type	Key features
Case 1	Once-through	Large LEU-fueled PWRs
Case 2	Once-through	Medium NU-fueled HWRs
Case 5	Once-through	B&B SFRs with DU makeup fuel
Case 7	Limited	LEU-fueled PWRs with Pu recycled to fuel EDSs
Case 10	Continuous	BWRs with TRU oxide fuel recycled with thorium
Case 13	Continuous	Fluid-fueled MSR with thorium makeup

7.1 Nuclear material accounting structures

To generate Code-10 style nuclear material accounting reports using Cntaur, an MBA file must be created for each case to bridge the Cyclus simulation agents and SSAC structures for nuclear material accounting at each facility that would be under safeguards. Standard accounting structures were developed to effectively model nuclear material accountancy and limit inter-case variation.

The library used to model nuclear fuel cycles for all case studies, Cycamore, is comprised of low-fidelity models. While they can be chained together to produce the relevant nuclear materials and used for work in system dynamics, they should not be mistaken for high-fidelity chemical process models. It is not possible to replicate a full accounting structure, which can have a dozen or more inventory KMPs and flow KMPs for some facilities.

In all cases, facilities were designed with a realistic number of MBA. One or more Cyclus agents are deployed per MBA to ensure that inventory changes are simulated as transactions and available for conversion to a Code 10-style ICR. Core inventory and flow KMPs are developed from model FAs or other model nuclear material structures published by the IAEA where available.

7.2 Behaviors and time fidelity

To meet the fidelity for fuel cycle simulations in safeguards applications, time steps of one day are required. While nuclear facilities typically record the hour and minute of a nuclear material inventory change, the accounting reports used in international safeguards must only have the day the change occurred. Cyclus and other nuclear fuel cycle simulators are typically used with time steps of one month or longer. Adjusting simulations down to time steps of one day requires adjusting temporal parameters for all agents such as throughput and inventory.

Consider the example State from Case 1 with one-day time steps. A second version of this case was created without any of the new capabilities described in Chapter 4, and a third version was also created without the new capabilities and with the simulation scaled back to approximately one month (exactly 30-day) time steps.

For the simulation cases without packaging capabilities, the size of fresh fuel shipments corresponds to either the full request amount or is governed by the constraining parameters of upstream facilities when resource constraints exist. When not resource-constrained, the shipment amounts are the full batch of assemblies. They cannot be accounted for individually as the transaction is made as a single bulk material.

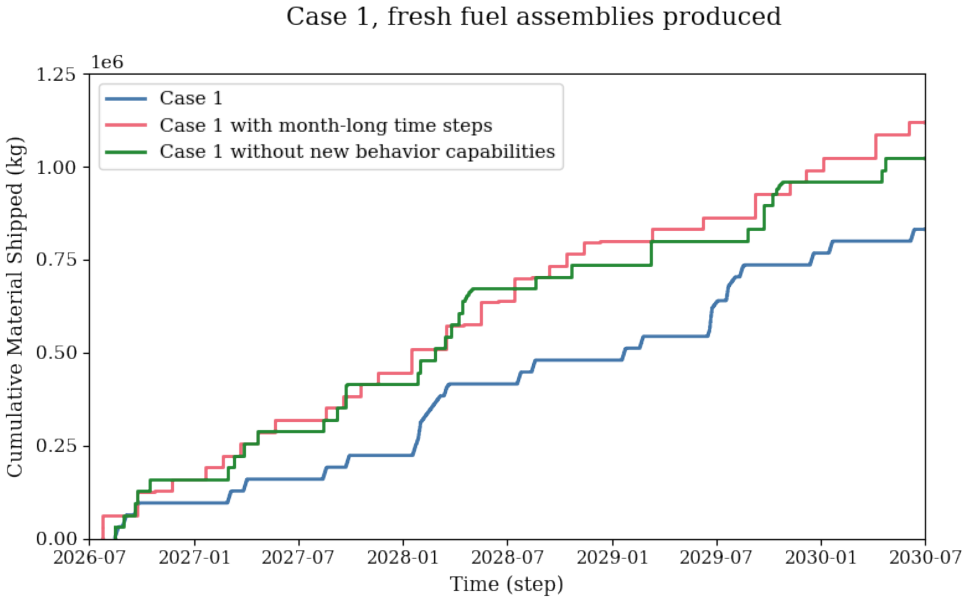

Figure 7.1: The new capabilities allow simulations to run with a just-in-time strategy. Compared to the cases without the new behaviors, the total material movement appears delayed. In effect, the other cases are unrealistically stockpiling material.

When resource constraints exist, such as if multiple reactors are refueling at the same time and requesting more material than can be produced each time step, material is shipped as fast as it can be produced. Production rates are subject to the constraints of each upstream agent that comprises the fuel fabrication facility and other contributing facilities.

All three systems can move enough fresh fuel for all reactors to refuel on time. Compared to the two simulations without new capabilities, Case 1 appears to be

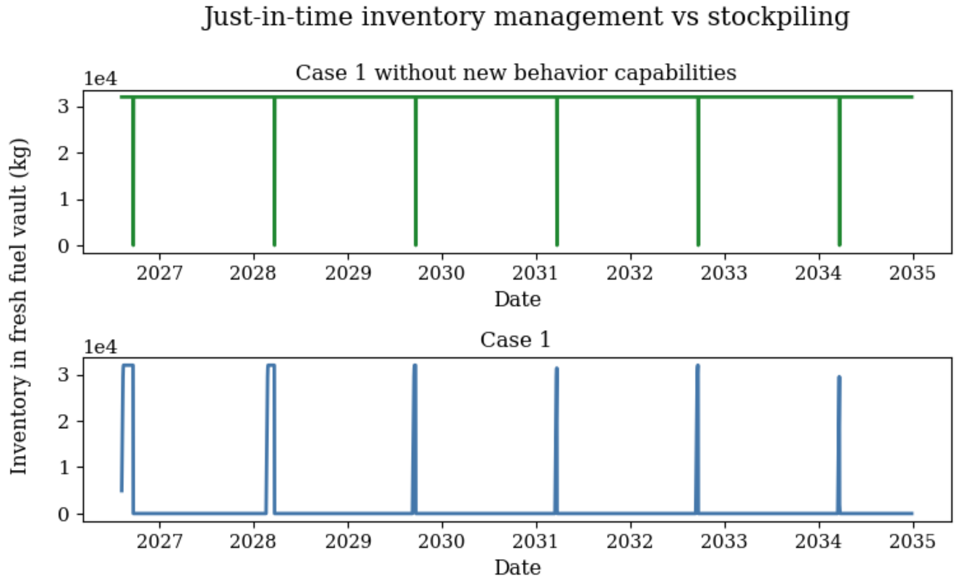

Figure 7.2: New capabilities like cumulative capacity allow agents that should remain empty, like fresh fuel vaults, to do so.

behind in total material shipped from the fuel fabrication facility. This can be seen in Figure 7.1.

The other simulations are ahead, and the simulation of Case 1 with all new behaviors is employing a more just-in-time (JIT) strategy by only ordering material when it is needed, shortly before the next cycle begins. The fresh fuel vaults for both simulations without the new cumulative capacity limits request material for the next cycle as soon as the current one begins, because their inventories have just been emptied. This can be seen in Figure 7.2, which shows the step-by-step inventory in a single fresh fuel vault throughout the simulation. The top figure, using the cumulative capacity feature, can maintain a JIT-like posture where material is only requested a few weeks before the outage begins. The length of the dormant period is also sampled from a normal distribution, introducing a bit of variability into the exact day that the fuel is requested and transacted into the reactor facility.

The simulations without the cumulative capacity capability, shown in the lower half of Figure 7.2, hold its fresh fuel for a full cycle length. The very next time step after loading fuel into the reactor core, new fresh fuel is requested (and received), moving the demand forward in time from when real nuclear power plants of this type should receive their next cycle's fuel.

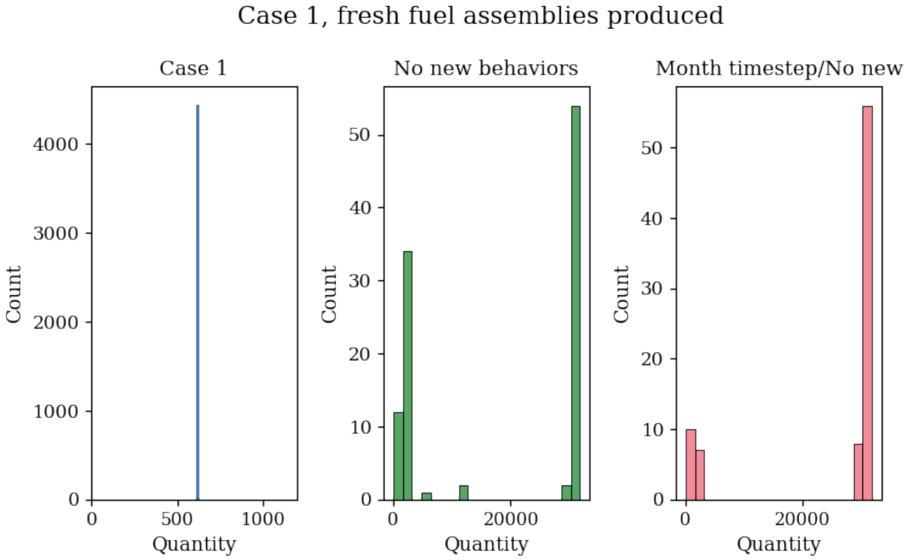

Figure 7.3: With item packaging, all shipments are exactly the size of the fuel assembly, and there are many more shipments. Without, packages are either the full request amount (largest bin) or correspond to the resource constraints of the producing agent.

In the packaging case, both shipment frequency and shipment size have meaning. Multiple shipments are made at the same time step because each shipment represents an individual, realistic nuclear material package. The total amount shipped per time step has meaning too, when transport units are employed. The shipment frequency reflects the production rate of the material. For the other two cases, it is only the shipment size that has meaning, it reflects the smaller of the material's production rate or the demand size. The shipment frequency is essentially one time step; as long as any amount of material is available, it will be shipped. This can be seen in Figure 7.3.

7.2.1 Simulation disruptions

Modeling changes and disruptions over time to a fuel cycle are one of the useful capabilities of a dynamic nuclear fuel cycle simulator. Disruption is a neutral way of representing a facility outside typical operation. In the context of this work, it only represents a facility that is not behaving within its typical buying pattern. It may also be used as a proxy for undeclared nuclear material processing. When processing is not happening "on the books", it could be happening with material that moves through the facility undeclared from start to finish. This work does not differentiate between disruptions where the facility is truly offline and disruptions where undeclared processing is occurring.

The effect of a disruption on a bulk facility depends on the length of the disruption and the slack in the facility. Facility disruptions are typically modeled at the beginning (receipt of feed materials) or ending (shipment of products) agent. Because a facility comprises multiple independent agents, there is no capability to disrupt all agents at once.

Two types of disruptions were injected into the front end of the fuel fabrication facility in Case 5. The long disruption is a full year, occurring only once in the 10-year simulation. The short disruption occurs more frequently but only lasts approximately one month. Both cases have the same expected total disruption, with the frequency varied inversely to the disruption length. The facility in the regular case simulation has the typical excess inventory storage, storing several batches worth of nuclear assemblies because domestic demand is seasonal but production occurs year-round.

Figure 7.4 shows the base Case 5 simulation against simulations with small or large disruptions, with and without restricted inventories. The restricted-inventory

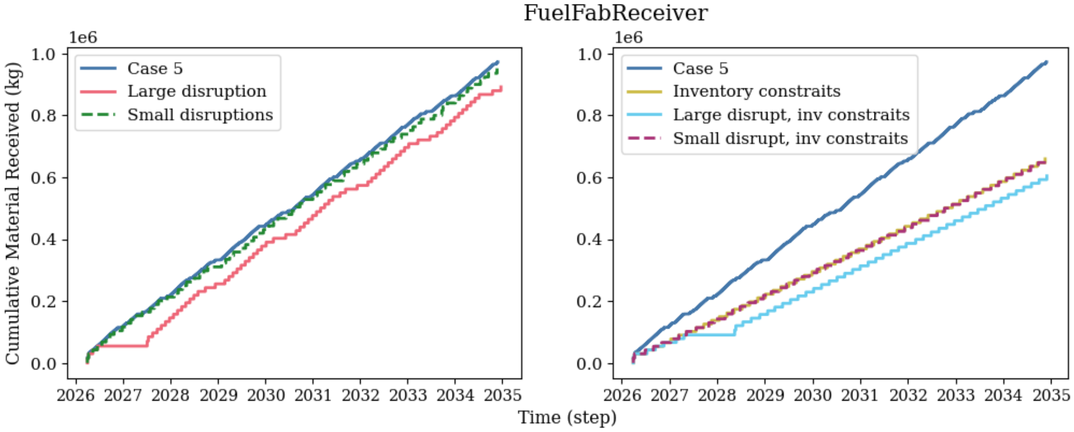

Figure 7.4: The length of disruption and the relative slack in the system affect whether the facility can ever catch up to the non-disrupted total production. Simulations on the left have typical inventory sizes, while simulations on the right have small inventories, leading to little slack in the system.

simulations can store less than a batch of fuel, preventing stockpiling when demand is not present.

On the left are simulations without restricted inventory. In this case, a large disruption prevents shipments of fresh fuel from going out on time. The entire system is delayed, and therefore the total shipments are always behind the base scenario. The small disruptions occur six times, but each disruption is short enough that production catches up each time. No reactors are delayed and the entire system is not affected.

The inventory-restricted simulations force the fuel fabrication facility into a resource-constrained position. The actual fuel production capacity is not restricted and remains adequate for the demand of 10 reactors, but the demand profile is not evenly distributed throughout the year, and therefore, the inability to store large quantities of fuel prevents these simulations from meeting the total demand. Similar to the regular inventory simulations, the small disruptions do not measurably impact the total amount shipped. The fabricator can recover to the no-disruption case by filling its assembly storage in time for the next demand wave. The large disruption

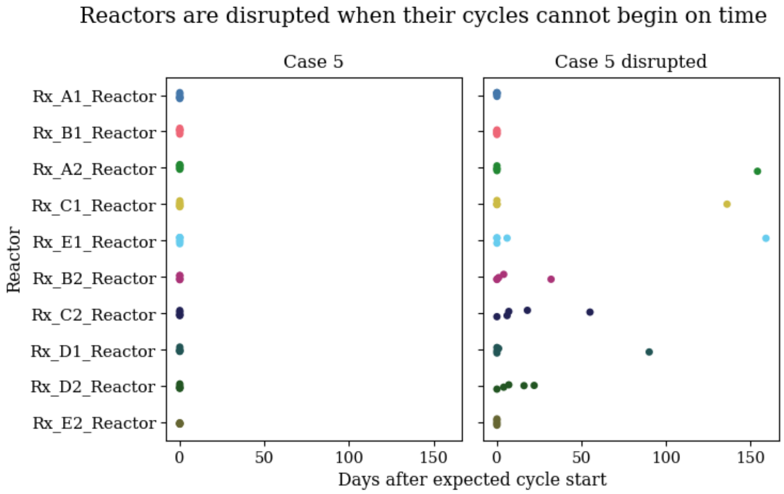

Figure 7.5: Several reactors are affected by the long disruption, causing their cycles to start later than expected.

prevents several reactors from coming online, delaying the entire system. When reactors cannot receive their fuel on time, their cycle is pushed back a corresponding amount forever.

When the disruption propagates down the fuel cycle, it can be seen in the behavior of the reactors. Figure 7.5 includes fresh fuel receipts for three reactors in the base case and with the long, one-year disruption. Inventories are not restricted.

The disrupted simulation does not affect the reactor outage for the first reactor, A1 (MBA GGA1). By the time fresh fuel is needed, the fabricator has recovered from its disruption. However, several other reactors need material during the disruption or the recovery period. Their receipt of fuel is delayed, and their cycles are also permanently pushed back.

More simulations with the same expected disruption can show the length of time at which the facility is no longer able to recover. Figure 7.6 shows the distribution of fuel assemblies shipped by the fuel fabricator at the end of the 10-year simulation for 50 simulations–30 with no disruption but different random seeds and 20 with disruption lengths ranging from 10 days to 1.5 years and frequencies varied to keep the expected total disruption fixed.

The boxplot shows the distribution of non-disrupted cumulative fresh fuel shipments, given the randomness built elsewhere into the system. When one or more longer disruptions occur but the system can still recover such that it ships enough fuel assemblies to lie within the bounds of the box plot, the system is said to recover. At some point, the disruptions get long enough that there is not enough slack in the system to recover even if they are correspondingly less likely to occur. For the system in Case 5, this point is between 180-210 days.

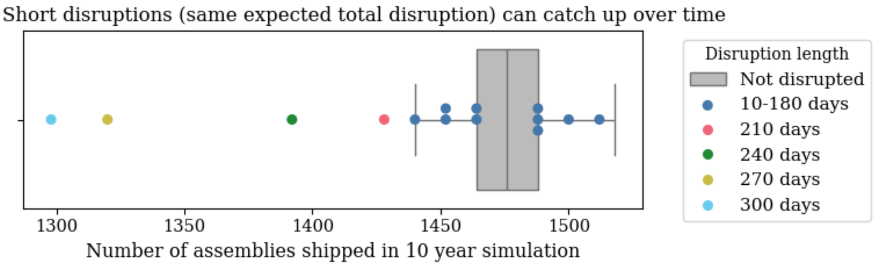

Figure 7.6: Whether or not a disruption causes a permanent delay to the system depends on disruption length, given a fixed expected total disruption.

This analysis is necessarily contrived; production of fresh fuel assemblies are completed under multi-year contracts between fabricators and reactors, not through a daily open market like Cyclus represents. However, disruptions would still propagate through a system but the pattern of throughput and storage would be governed by the known upcoming demand rather than fixed values.

This capability is generalizable. Any fuel cycle could be analyzed in this way by generating many versions of the same system, both disrupted and not, evaluating the impact of the disruption within the bounds of the expected system variation.

7.2.2 Reactor accounting structure

There are three standard reactor accounting structures, based on the movement patterns of nuclear fuel into and out of the core. All reactors used in the case studies are categorized as either off-load, on-load, or fluid fueled as shown in Table 7.2.

Table 7.2: Reactor MC&A type for each fictitious State

	Type of reactor		
Case	Off-load reactor	On-load reactor	Fluid-fuel
Case 1	✓		
Case 2		✓	
Case 3		✓	
Case 4	✓		
Case 5	✓		
Case 6	✓		
Case 7	✓/✓		
Case 8	✓		
Case 9	✓		
Case 10	✓		
Case 11	✓/✓		
Case 12	✓(St1)	✓(St2)	
Case 13			✓

First is reactors that refuel only during a refueling outage, where the reactor is shut down and not producing power. The structures for these reactors are based on an IAEA safeguards technical report, *Detailed Description of an SSAC at the Facility Level for Light Water Moderated (off-load refueled) Power Reactor Facilities* [160]. The reference reactor is a PWR with LEU, but the same principles are applied to other reactor designs that have the same refueling strategy.

These reactors all have a single MBA for the entire facility, regardless of the number of reactors at the power plant. The nuclear material accounting structure for these reactors is shown in Figure 7.7. The reactor designs used in Chapter 6.4 that are considered off-load are PWRs, BWRs, heat-pipe reactors, SFRs, and EDSs.

Material arrives at the reactor at flow KMP 1 and inventory KMP A, which in Cyclus is modeled as a single agent representing the receiver area and fresh fuel vault(s). Fuel does not cross MBA boundaries, only inventory KMP boundaries when being loaded into the core. When the fuel is permanently discharged into the UNF pool, two inventory changes are recorded for the nuclear loss and nuclear production at flow KMP 2 and inventory KMP C. Finally, when the used fuel is shipped off-site, the change is recorded in flow KMP 3. No other movements of fuel trigger an inventory change, including the loading of used fuel into MPCs for dry storage.

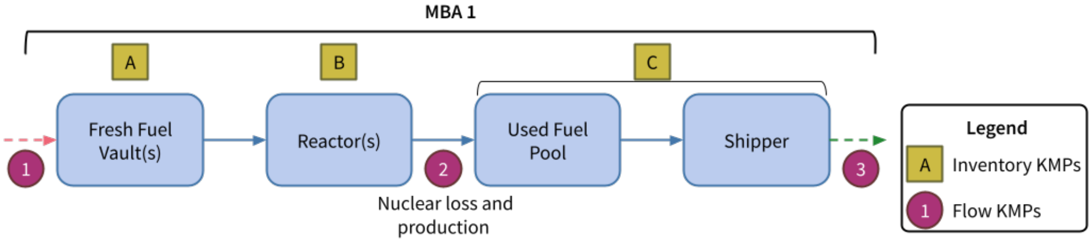

Figure 7.7: MBA and KMP structure for both off-load and on-load reactor types

Another group of reactors is solid-fueled reactors which refuel during operations. The structures for this type of reactor are based on a similar IAEA report for on-load reactors, *Detailed Description of an SSAC at the Facility Level for On-load Refueled Power Reactor Facilities* [161]. The reference design is a 600 MWe CANDU, similar to Case 2.

These reactors refuel much more frequently than off-load reactors but have a very similar nuclear material accounting structure. The only difference is that fuel bundles are discharged individually to a smaller storage area before being moved into long-term cooling and storage. Two reactor styles fall in this category, HWR and TRISO-fueled pebble-bed reactors.

For HWRs, fuel bundles are discharged from the reactor into a storage rack in the discharge bay. When the storage rack is full, it is transferred to a larger UNF storage pool. However, the storage racks used in CANDU reactors have the same capacity as the daily discharge of fuel, 24 bundles. The movement from the discharge bay to the storage pool is assumed to occur on the same day as the fuel was discharged from the reactor core and therefore is captured by the existing process flow of the reactor agent.

The TRISO pebbles flowing through a HTGR are cycled at a rate much higher than the charge/discharge rate. The reference design for Case 3 is the HTR-PM reactor, which cycles 6,000 (out of 420,000) pebbles each day but only discharges approximately 400 pebbles based on burnup [162]. The pebble cycling is not modeled–only the discharging process is included in simulations. Therefore, this design can also adequately be modeled using the simulation agent-nuclear material accounting structure shown in Figure 7.7.

The last standard group of reactors has fluid fuel that is moving in and out of the core continuously. There are no fluid-fueled reactors currently under IAEA safeguards, so the nuclear material accounting structures for a fluid-fueled reactor are still theoretical.

Several recent reports, one by Shoman and Higgins at Sandia National Laboratory (SNL) [163] and several from ORNL including Dion and Hogue [164] and Hogue *et al.* [165], focus on developing potential material control and accounting/accountability (MC&A) structures under Nuclear Regulatory Commission (NRC) regulations. These same structures could also be used for nuclear material accounting for a State under international safeguards. Hogue *et al.* recommend that fluid-fueled MSRs not be treated like existing off-load reactors, on-load reactors, or bulk facilities, but have a new specialized MC&A approach, which they deem inventory-monitor containment-inventory (IMCI).

The IMCI approach places the continuous salt-treatment and chemical separation processes into the same MBA as the reactor. The receiving and storage of solid fresh fuel is in MBA 1, and the storage and shipment of wastes occurs in MBA 3.

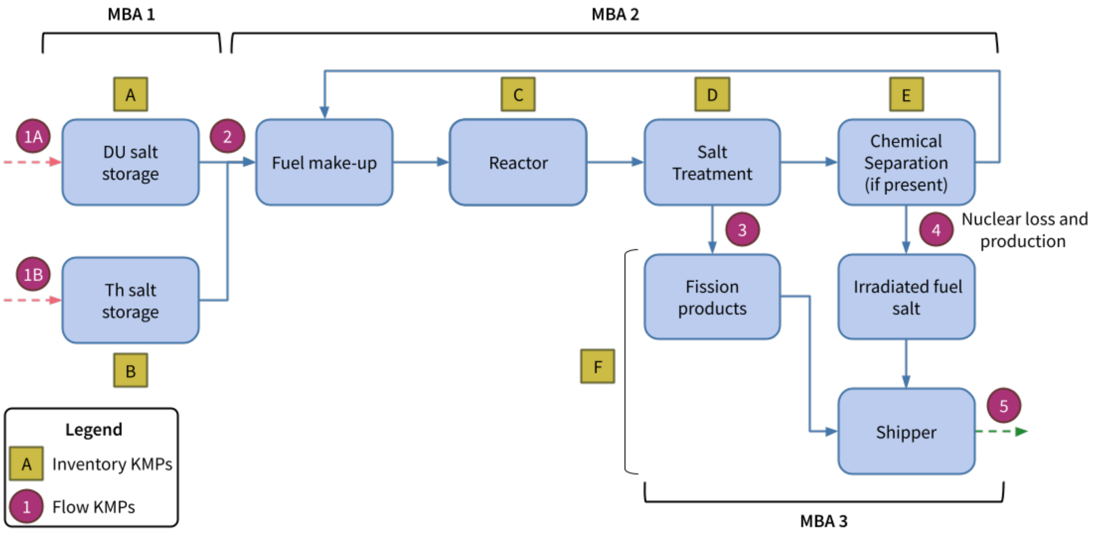

Figure 7.8: MBA and KMP structure for fluid-fueled reactors

There have been other MBA structure proposals. Arno at the University of Texas at Austin proposed MBA structures [166] that varied based on the reactor design, including a two-MBA and a three-MBA structure with different processes in each MBA than the IMCI approach. Armstrong at Texas A&M proposed an MBA structure for two-loop fluid fueled MSRs [167] that separated the reactor, fuel-salt treatment, and blanket-salt treatment each into individual MBAs. However, the three-MBA structure with a single "process" MBA continues to be mentioned in reports for the DOE Advanced Reactor Safeguards & Security program [168], so this structure is used for cases with fluid-fueled reactors.

7.2.3 Front end facilities

Mining and milling of uranium and thorium occur before the starting point of safeguards, so no nuclear material accounting structures were developed or used.

The conversion facility producing UF_6, UO_2, or other chemical forms has an MBA structure developed from a version of the IAEA's *Model Facility Attachment for Conversion Plant with Three Parallel Process Areas* [169]. This model is more generic than existing plants, assuming that a single facility may process NU, DU, thorium, LEU below 5% enrichment, and HALEU. MBA2 is designated for the natural and lower uranium enrichments and thorium, MBA3 is for processing LEU below 5% enrichment, and MBA4 is for HALEU. The generic MBA structure in Figure 7.9 reflects these structures, although no simulated conversion plants contain MBAs 3 and 4 because conversion from enriched UF_6, often referred to as deconversion, is modeled as a process within a fuel fabricator.

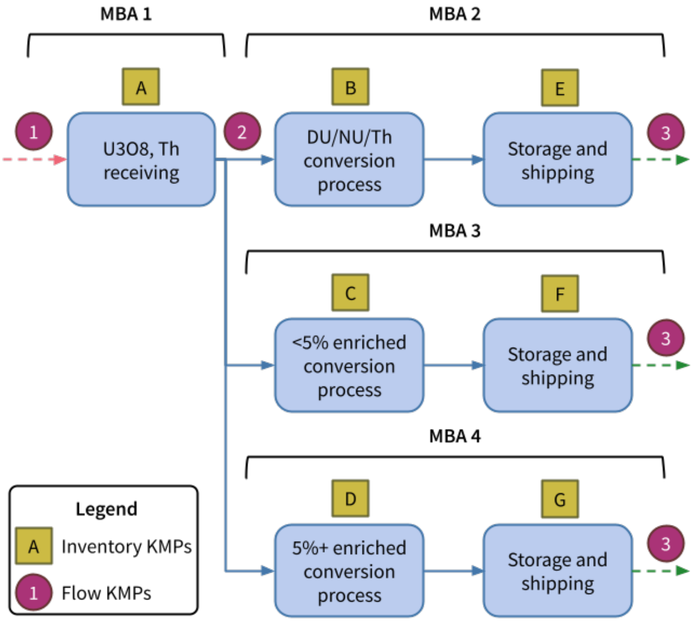

Figure 7.9: MBA and KMP structure for chemical conversion plants

MBA2 has the same nuclear material accounting structure regardless of the chemical form created, from UF_6 for enrichment to natural UO_2 for HWRs to ThF_4 fuel salt for MSRs.

An IAEA report, *International Safeguards in the Design of Enrichment Plants* [170] recommends up to four MBAs for a gas-centrifuge enrichment plant, with the four areas described as "The receipt and shipment of nuclear material; In-process nuclear material; Analytical, weighing and sampling activities; Waste and other material." Enrichment facilities are modeled without weighing and sampling activities, and following the assumptions made by the DOE Fuel Cycle Options Campaign Evaluation & Screening report [111], no waste or process losses are included either. Figure 7.10 shows how as a result of the modeling choices, enrichment facilities are modeled with just two MBAs. The cylinder storage areas where receiving and shipping occur, as well as long-term DU storage if the material is not otherwise being used, are both in MBA1.

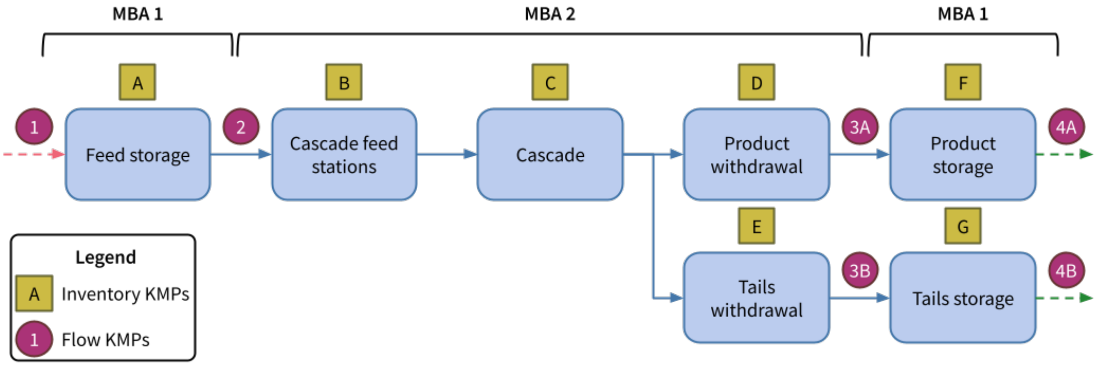

Figure 7.10: MBA and KMP structure for centrifuge enrichment plants

Nuclear material accounting structures for fuel fabrication facilities, including (de)conversion when applicable, are based on an IAEA report, *Detailed Description of an SSAC at the Facility Level for a Low Enriched Uranium Conversion and Fuel Fabrication Facility* [171, 172], as shown in Figure 7.11.

When relevant, deconversion from UF_6 to the appropriate fuel form is included.

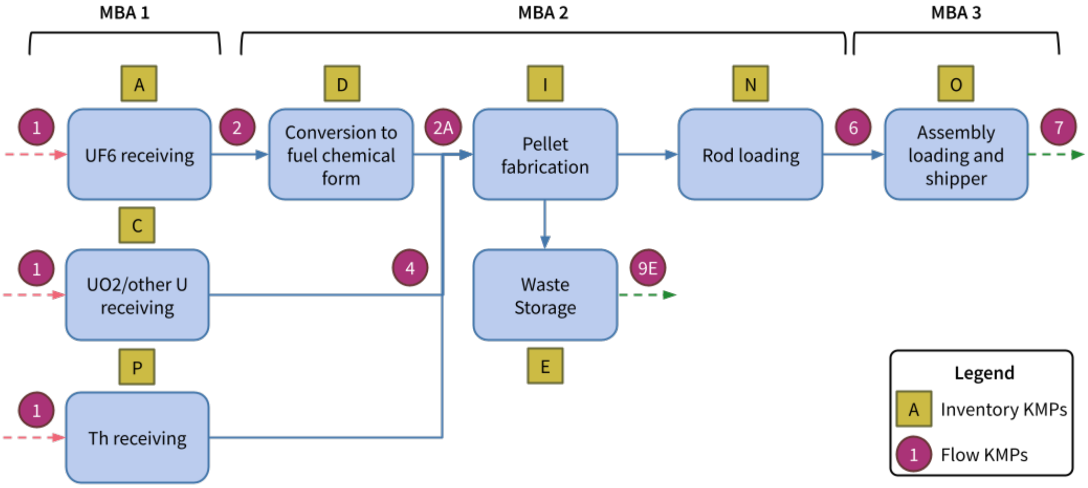

Figure 7.11: MBA and KMP structure for fresh fuel fabrication and deconversion

7.2.4 Back end facilities

There have been several published approaches to defining nuclear material accounting structures for reprocessing plants. Smaller plants may consider using as few as three MBAs, such as the one described for a model plant producing 200 tons/year in a report jointly published by the IAEA, Japan Atomic Energy Research Institute (JAERI), and Japan's Power Reactor and Nuclear Fuel Development Corporation (PNC) [173].

The Rokkasho reprocessing plant in Japan, the only commercial-scale reprocessing plant in a NNWS under construction or operation, is designed to produce 800 tons per year and has five MBAs [174]. This aligns with the current guidelines from the IAEA in the design of new reprocessing plants under safeguards recommend four MBAs unless TRU powders like PuO_2 will be produced in the facility, and then at least a fifth MBA is recommended, or other "[m]ore complex MBA structures" [14]. All of the previous approaches are specific to the PUREX process that was first developed in the 1950s and is the only reprocessing technique currently in commercial use. Other structures are proposed for novel reprocessing techniques,

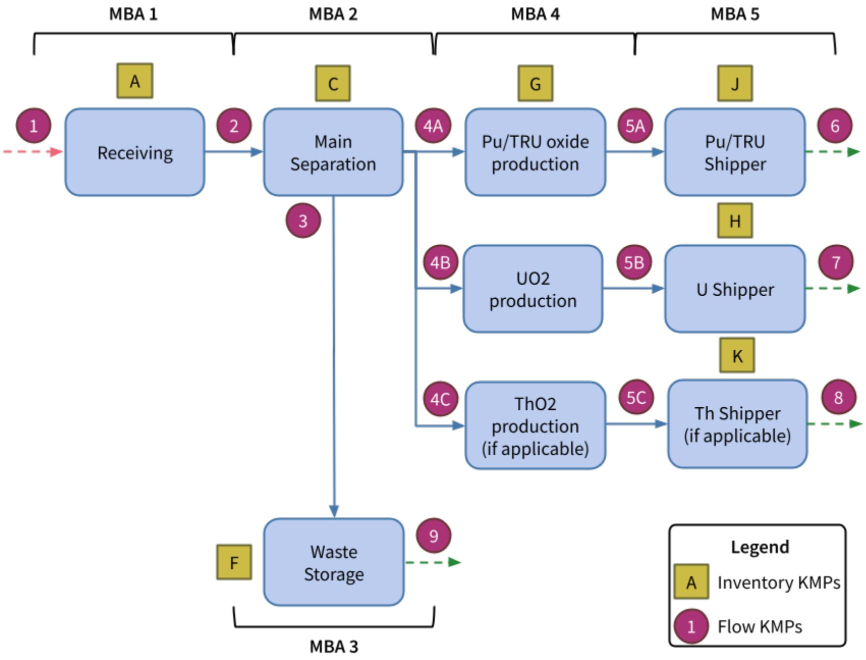

Figure 7.12: MBA and KMP structure for reprocessing plants

such as a report by Durst *et al.* at PNNL which developed a six-MBA facility [175].

Reprocessing modeled in the case studies does not differentiate between separation processes. Therefore, the structure similar to IAEA reference design, the Rokkasho plant, is used for plants that produce TRU products as shown in Figure 7.12. Reprocessing facilities are always assumed to be separate from recycled/mixed-actinide fuel fabrication, although they could be co-located for ease of material movement. MBA4 of a reprocessing plant will always produce the chemical form needed to fabricate recycled fuel.

The recycled fuel fabrication plant, in Figure 7.13, was modeled after "Detailed Description of an SSAC at the Facility Level for Mixed Oxide Fuel Fabrication Facilities" [176]. The facility looks similar to the fresh fuel fabrication plant except no deconversion is included and the incoming materials are already in the fuel chemical form.

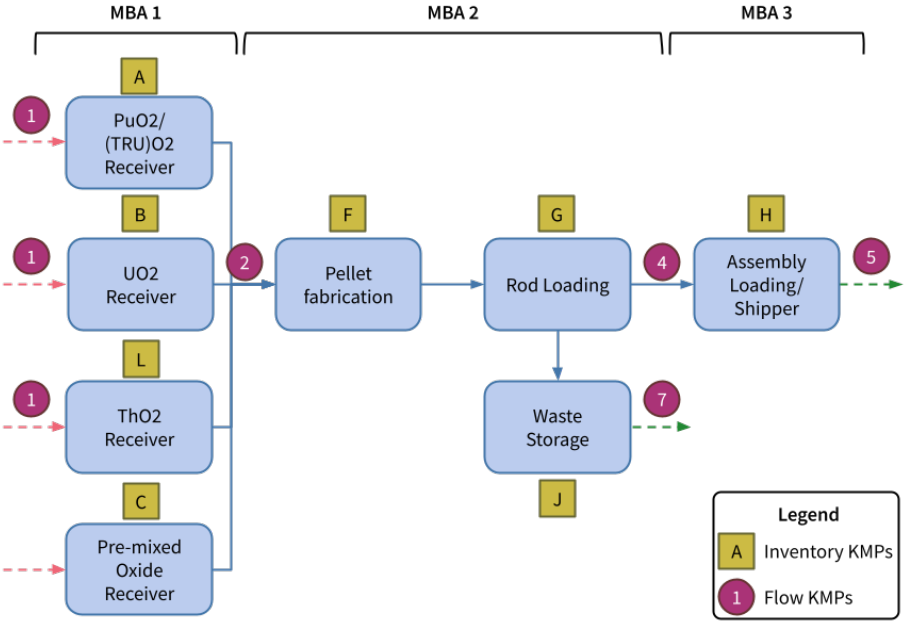

Figure 7.13: MBA and KMP structure for recycled fuel fabrication plants

CIS facilities have two MBAs as shown in Figure 7.14. Long-term storage is the final step of any case study, permanent disposal pathways are not included. Unlike disposal facilities where termination of safeguards would be possible for materials entombed in an irrecoverable manner, in CIS nuclear materials remain under safeguards and would be eligible for inclusion in regular PIL reports.

Because CIS facilities are the last step of the NFC for any of the case studies, there is no flow KMP or shipment out of the CIS. In a real system, nuclear materials could eventually move to a final disposal facility, or to a reprocessing system for reuse.

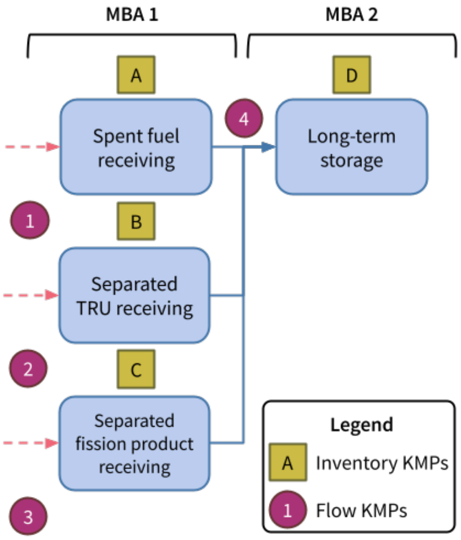

Figure 7.14: MBA and KMP structure for consolidated storage facilities

7.2.5 Other facilities

Research reactors follow a *Model Facility Attachment for Research Reactor IRT/VVR-S* [177] with only one MBA. One key difference for research reactors compared to power reactors for the training and zero-power reactor is that a separate UNF pool is not included as a simulation agent or as an inventory KMP. An additional UNF pool and inventory KMP-C are added for the medical reactor, which refuels frequently. In either case, nuclear loss and production and shipment of nuclear material off-site are recorded with the same flow KMP, KMP-2.

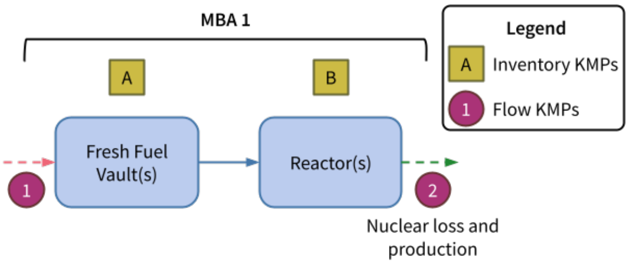

Figure 7.15: MBA and KMP structure for training and zero-power research reactors

7.3 Code 10

Labeled Code 10 ICRs were created for each of the demonstration cases listed in Table 7.1, using the MBA structures developed in Section 7.1. Simulations run for ten years by default, but some were shortened due to memory issues on the laptop used to generate the Code 10 reports.

7.3.1 Realistic entry numbers and weights

Packaging is an essential component of generating realistic Code 10 reports. Without realistic quantization of materials, entire batches of nuclear materials are transacted in single quantities, often tens of tons at a time, for simulations that aren't resource-constrained. Where resources are constrained, and demand for fresh fuel outstrips supply, materials are shipped in unrealistic quantities as soon as they are produced. For example, a fuel fabrication plant with an annual production capacity of 750 tU/year would produce a maximum of 2,337 kg UO_2 per day. For a plant producing LWR-style fuel assemblies, this results in about 3.8 assemblies shipping per day, or 107.3 bundles per day for HWR-style fuel. These amounts are the maximum and are not fixed, so resource constraints could also result in three consecutive fresh fuel shipments of 1.1, 3.1, and 2.7 assemblies, none of which are useful when trying to model a realistic system with realistic nuclear materials because fuel assemblies only exist in integer quantites.

Consider the receipt of fresh fuel for three water reactors. Case 1 with LEU fuel, Case 2 with NU fuel, and Case 10 with thorium, RU, and TRU fuel.

The simulated data that would be available without any of the new capabilities from Chapter 4, if they were converted to Code 10 inventory change reports, is much more limited. For Case 10, the receipt of a batch of 52 fuel assemblies would only appear as a single entry with a single item having the batch aggregated mass as its quantity. Accordingly, the weight labels 630 and 670 are for the entire batch. This report would not be appropriate without the new capabilities because it would not be possible to independently account for individual fuel assemblies.

This report would also be unable to reasonably define some other required Code 10 labels, such as 430 MDC. Defining a blended mass as one singular fuel assembly is not acceptable. Bulk quantities must be declared by the volume of their containers; items are declared by their type. A single bulk quantity of over 28 tons of enriched uranium is neither based on a realistic container volume nor a meaningful item (it is not realistic). But the individual assembly receipt with the new packaging capability can correctly be declared with the physical form `B`, corresponding to "Fuel elements. Complete fuel elements for a given reactor system (e.g. assemblies or bundles)". Code listing 7.1 gives a single ICR report entry for a single fuel assembly receipt from Case 1 in labeled Code 10 format and Table 7.3 expands the single entries from Cases 1, 2, and 10 into a more intuitive format.

```
001:OI/CC;1#002:1/312#003:20250530#006:TEST,TEST#010:I#015:20250401/20250430#207:
    CCB-#307:CCB1#309:N#310:49109#370:AA/AA#372:CC/CCB1#407:1#411:RF
    #412:20250406#430:B/Q/2/F#436:startup_LEUO2_fuel#446:256086#447:256086#469:N
    #470:1#630:542282.2G#670:26029.9G#
```

Listing 7.1: Single entry of a Code 10 report representing the receipt of a fresh fuel assembly in Case 1 (MBA CCB1). The weight labels include 630 Enriched Uranium and 670 U-235.

All three cases are water-cooled reactors, but their differences are reflected in the report entries. Case 1 reactors are fueled with 156 assemblies. Two of the PWRs, both within the same MBA of CCB1, received fuel this month for a total of 312 entries.

Similarly, for Case 2 the prior modeling capabilities are inadequate for the task

Table 7.3: Code 10 snippets for Cases 1, 2, and 10 during initial fresh fuel receipt

#	Title	Case 1	Case 2	Case 10
001	Reference #	OI/CC;1	OI/DD;1	OI/NN;1
002	Entry # / Total	1/312	1/8844	1/720
003	Report Date	20250530	20250302	20250302
006	Encoder's name	TEST,TEST	TEST,TEST	TEST,TEST
010	Report Type	I	I	I
015	Report Period	20250401/20250430	20250213/20250228	20250102/20250131
207	Facility Code	CCB-	DDB-	NNA-
307	MBA Code	CCB1	DDB1	NNA1
309	Entry Status	N	N	N
310	State Record ID	49109	132663	6284
370	Shipper	AA/AA	AA/AA	AA/AA
372	Receiver	CC/CCB1	DD/DDB1	NN/NNA1
407	KMP Code	1	1	1
411	Type of Change	RF	RF	RF
412	Date of Change	20250406	20250213	20250102
430	MDC	B/Q/2/F	B/Q/2/F	B/Q/2/F
446	Batch Name	256086	605244	38797
447	Shipper's Batch	256086	605244	38797
469	Measurement	N	N	N
470	Number of Items	1	1	1
610	Natural U		19.2K	
630	Enriched U	542282.2G		139461.3G
660	^{235}U + ^{238}U Content			9286.1G
670	^{235}U Content	26029.9G		
700	Plutonium			18236.5G
800	Thorium			114.22K

at hand. In a given month, say March 2025, nuclear fuel is both received at a HWR facility and discharged from the reactor. The HWRs in Case 2 receive fuel annually. In the old simulation without packaging capabilities and dormant periods, this would appear on a Code 10 report as only 73 entries. One entry corresponds to the bulk receipt of a year's worth of fuel bundles as a single mass. The other entries are individual bundles being discharged from the reactor and receipt of new fuel assemblies because the fresh fuel vault attempts to maintain a full inventory each day. With the new capabilities, the reactor receives 8,748 fresh bundles plus two days of operation resulting in 48 bundles discharged. Each discharged bundle creates two entries, one for nuclear loss and one for nuclear production, resulting in a total of 8,844 entries. Finally, one BWR in Case 10 receives a full core of material, 720 assemblies. All are fresh fuel assemblies received in a shipping container, so they all have an identical 430 Material Description Code.

Weight labels also distinguish the fresh fuels from each other. The LEU assemblies in Case 1 are large, with over 500 kg of enriched uranium. Due to the enrichment, the weight data is reported with 630 Enriched Uranium and 670 Uranium-235 Content labels, both in grams. Because the HWR bundles in Case 2 contain only NU, their weight is reported only with 610 Natural Uranium, in kilograms. Finally the recycled fuel in Case 10 contains both ^{233}U and ^{235}U, so label 660 was used instead of 670. Plutonium from the recycled fuel necessitates 700 Plutonium in grams and the makeup fuel is thorium, which adds label 800 Thorium in kilograms.

7.3.2 Realistic entry frequency

Several case study reactors have very short effective cycle lengths. Case 2 discharges fuel bundles each day, and the fluid-fuel MSR modeled in Case 13 is modeled as discharging some fuel salt every ten days, which is the cycle length.

With the prior one-month timestep, high cycle length reactors and facilities with frequent inter-MBA transactions would not be able to distinguish between a material moving on the first day and the last day of the month. With one-day timesteps, movements can be recorded on the day they occur. Listing 7.2 shows the first nuclear loss entry from discharged fuel bundles on three consecutive days for a reactor in Case 2 using label 412 Date of Inventory Change. The first and last entries are only two days apart, but they span two months and, therefore, are part of two different reports, which can be seen in label 001 Reference Number. The first two entries, in January, are part of report `OI/DD;1` while the third entry in February is part of report `OI/DD;2`.

```
001:OI/DD;1#002:8769/8844#003:20250302#006:TEST,TEST#010:I
    #015:20250128/20250131#207:DDB-#307:DDB1#309:N#310:142836#370:DD/DDB1#372:DD/
    DDB1#407:A#411:LN#412:20250130#430:B/Q/1/G#436:NatUO2_fuel_B1_spent
    #446:749968#447:749968#469:N#470:1#610:0.2K#
...
001:OI/DD;1#002:8797/8844#003:20250302#006:TEST,TEST#010:I
    #015:20250128/20250131#207:DDB-#307:DDB1#309:N#310:143319#370:DD/DDB1#372:DD/
    DDB1#407:A#411:LN#412:20250131#430:B/Q/1/G#436:NatUO2_fuel_B1_spent
    #446:751475#447:751475#469:N#470:1#610:0.2K#
...
001:OI/DD;2#002:1/1344#003:20250330#006:TEST,TEST#010:I
    #015:20250201/20250228#207:DDB-#307:DDB1#309:N#310:143786#370:DD/DDB1#372:DD/
    DDB1#407:A#411:LN#412:20250201#430:B/Q/1/G#436:NatUO2_fuel_B1_spent
    #446:752966#447:752966#469:N#470:1#610:0.2K#
```

Listing 7.2: Nuclear loss is an inventory change recorded when a fuel bundle is permanently discharged, along with the corresponding nuclear production. For a HWR in Case 2 that discharges fuel each day (MBA DDB1), this results in daily entries. Here are three discharges on consecutive days, note how the third entry is captured by a different report.

7.3.3 Domestic and foreign receipt

ICRs naturally evolve as the system reaches steady state. Report #1 shown in Listing 7.1 correctly identifies that fuel shipment as having a foreign origin in label 411 Type of Inventory change as `RF`, "Import of nuclear material into Country". This is a modeling choice, as foreign fuel is imported at higher rates than would be available domestically to start up reactors on their designated deployment dates. However it also demonstrates the appropriate categorization, as the makeup fuel source used in the simulation was assigned a foreign origin. Later in the simulation, enough fuel is available from the domestic power plant. The fuel is shipped from fabricator MBA CC23 as declared in label 370 Shipper of Nuclear Material, resulting in an inventory change that is now domestic, `RD` or "Domestic receipt of nuclear material from another MBA".

This same swap for a single inventory change to be categorized as `RD` instead of `RF` could also be achieved with the same simulation but one change to the MBA file. In the standard process used to generate Code 10 reports from individual cases using CNTAUR, all processes not available within the country are designated to exist in a partner country, always fixed as country `AA`.

Even countries with fuel fabrication plants may not be able to process enough fuel to start up reactors all at once, which requires an entire new core of material and not just the typical order of a batch. To address this, the startup cores are always imported and assumed to be available exactly on demand. However if this source of startup fuel were instead assumed to be some cache of material within the country, and given the same country code, it would be tagged as a domestic receipt. Listings 7.3-7.4 show how this change would only require modification to the country and name of the MBA containing the startup fuel, from foreign `AA` to the domestic code `CC` in order to flip the inventory change code for all initial-core fresh fuel receipts.

```
<MBA>
    <country>AA</country>
    <name>AA23</name>
    <agents>
        <agent>Startup_Source</agent>
    </agents>
</MBA>
```

Listing 7.3: This MBA snippet produces shipments with the inventory change code RF

```
<MBA>
    <country>CC</country>
    <name>CC23</name>
    <agents>
        <agent>Startup_Source</agent>
    </agents>
</MBA>
```

Listing 7.4: This MBA snippet produces shipments with the inventory change code RD

Running the same simulation, Case 1, and flipping the country of the initial core source results in two nearly identical sets of reports, shown in Table 7.4. One entry from report `OI/CC;4` of MBA `CCB-` looks identical except for the 370 Shipper of Nuclear Material and 411 Type of Inventory Change label.

Table 7.4: Switching the source of the initial core from external country AA to the domestic country CC changes the shipper of material as well as the type of inventory change the entry is categorized as

#	Title	Fuel Source		#	Title	Fuel Source	
		AA	CC			AA	CC
001	Reference #	OI/CC;1		002	Entry # / Total	1/312	
003	Report Date	20261130		006	Encoder's name	TEST,TEST	
010	Report Type	I		015	Report Period	20261001/20261031	
207	Facility Code	CCB-		307	MBA Code	CCB1	
309	Entry Status	N		310	State Record ID	217339	
370	Shipper	AA/AA	CC/CC23	372	Receiver	CC/CCB1	
407	KMP Code	1		411	Type of Change	RF	RD
412	Date of Change	20261020		430	MDC	B/Q/2/G	
446	Batch Name	1146174					
447	Shipper's Batch	1146174		469	Measurement	N	
470	Number of Items	1		630	Enriched U	542298.8G	
670	^{235}U Content	26029.9G					

7.3.4 Recreating systemic patterns

One of the indicators of successfully turning Cyclus simulations into labeled Code 10 reports is to ensure that synthetic nuclear material accounting reports contain only and exactly the information that the IAEA receives from real reports.

One way to verify that all the relevant information from a Cyclus simulation is converted into accounting reports is to reproduce the patterns of nuclear material movement using the Cyclus simulation directly and by aggregating the labeled Code 10 reports across all months and across MBAs. Figure 7.16 sums the ^{235}U present in all the outgoing transactions by the shipper agent of any reactor in the Case 7 Cyclus simulation output on the left and sums all of the 670 ^{235}U Isotopic Content information shipments from the reactor MBAs in the ICRs on the right. The total amount is the same, within a small tolerance due to rounding in Code 10 reports, and the number of shipments are identical. All relevant transactions are being captured in the nuclear material accounting reports.

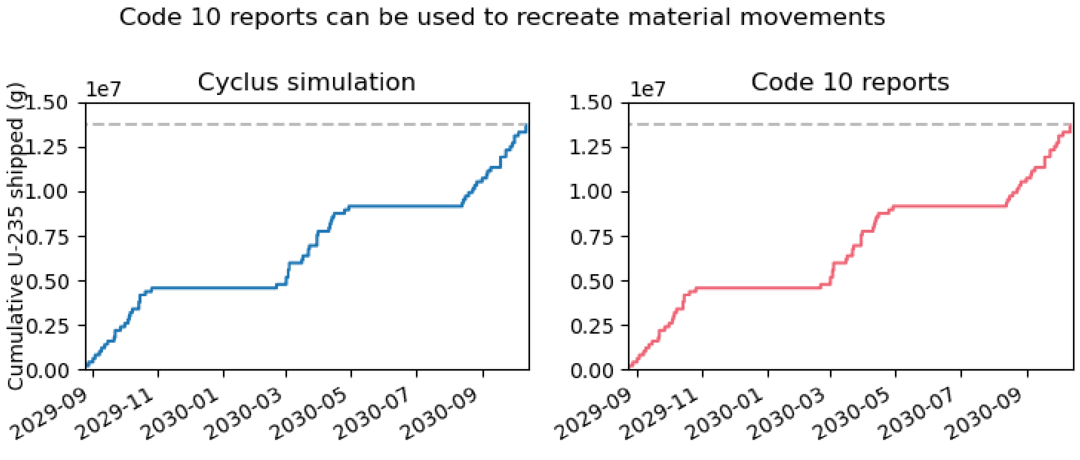

Figure 7.16: All of the information about ^{235}U in used fuel shipments in a Cyclus simulation is captured in the Code 10 reports

Core nuclear materials in the simulation like ^{235}U are fully captured, but some transuranics are not. Per IAEA Statute [178] as referenced in INFCIRC/153 (Corrected) [54], the relevant nuclear materials for nuclear material accounting are special nuclear materials and source materials, which collectively encompass uranium, thorium, and plutonium. Other nuclear materials, particularly neptunium and americium, are not included. While the IAEA does collect information on neptunium and americium through special monitoring schemes set up in conjunction with relevant States [2, 179], these are not captured through the regular nuclear material accounting reports.

This means that the only information about MAs in Code 10 reports is in the inventory change for nuclear loss, which is the estimated loss of mass due to all nuclear processes and includes the generation of plutonium, which is separately declared in nuclear production, and FPs and MA, which are not.

8 SUMMARY AND CONCLUSION

The fields of nuclear fuel cycle simulation and international safeguards both consider the movements of nuclear materials throughout the entire fuel cycle but have traditionally approached this process from different angles. This dissertation merges these two sub-fields with the recognition that careful expertise is required in both areas to avoid numerous pitfalls. Each chapter tackled a different aspect of this challenge, but they are linked in their focus on the fuel cycle as a system and not just a collection of individual facilities.

Chapter 3 was chronologically the first work undertaken. There has been a perception by safeguards practitioners that limitations with nuclear fuel cycle simulators made them of little use to the field. Some of the concerns raised mimic considerations detailed by Juchau *et. al*[21], including but not limited to the fact that most early simulators, and some still today, have limited ability to model facilities as individual units. Modeling dozens of reactors as a single fleet operating in unison with no dynamism does indeed restrict the usefulness to safeguards. Tracking nuclear materials as a bulk mass is not adequate for a detailed analysis of a nuclear energy system. The existing capabilities of Cyclus already included many of the capabilities desired by the safeguards community, so this work sought to apply to the needs of the safeguards community and then to identify the limiting factors of Cyclus and address them in the following chapters.

Chapter 3 was the first step in illustrating the usefulness of Cyclus to safeguards. By focusing on an existing methodology in the field, APA, this work demonstrates how the ecosystem of a nuclear fuel cycle simulator can be used to conduct safeguards analyses.

Next, the work in Chapter 4 addresses some of the capability gaps in Cyclus at the spatial and temporal fidelity required in international safeguards. Focusing on the inventory management tools available to agents to interact with the DRE allows all steps in the nuclear fuel cycle to leverage the new capabilities instead of focusing on a single facility type.

The new buying-side behaviors expand beyond the simple inventory scheme that any gap between the inventory limitations and current inventory should be filled. Buying restrictions were developed based on time, the cumulative amount received, and stochastic reductions in request size.

A packaging capability was developed, and the new selling-side behaviors implemented packaging on materials being offered to the DRE. Now users may define nuclear material packages and transport units based on the mass and quantity limitations relevant to their simulation. Several stochastic and deterministic packaging fill strategies allow for even more flexibility in using packaging to split and merge resources into realistic quantities as they move between agents.

With the new behaviors developed in Chapter 4, it is now possible to develop simulations with one-day time steps and to replicate movements of nuclear materials in realistic quantities. Chapter 5 developed a post-processing tool for CYCLUS simulations to convert the information into the exact style and format that NNWS Parties to the NPT must submit their nuclear material accounting reports, called Code 10.

The conversion tool, called CNTAUR, also blends the agents used in a fuel cycle simulation with the MBAs and KMPs that govern when formal inventory changes must be recorded on Code 10 reports.

Chapter 6 combined the development of country-sized fuel cycle models, common in nuclear fuel cycle simulation, with the consideration that a safeguards-focused dissertation should not use real countries out of concern for politicization, an ever-present issue in international safeguards.

Thirteen country-sized case studies were developed, with enough detail about the reactor system(s) and fuel cycle facilities that they could be developed into full simulations using Cyclus or another fuel cycle simulator.

Finally, Chapter 7 uses the new behavioral capabilities developed in Chapter 4 within several of the case studies from Chapter 6.4 to create a set of Code 10 ICRs on the level of an entire country over the course of several years. These new capabilities and tools within the Cyclus ecosystem can be used to demonstrate the impact of disruptions or other changes to the flow of nuclear materials across a State's entire fuel cycle.

8.1 Suggested future work

This dissertation identifies areas where nuclear fuel cycle simulators could be applied to international safeguards challenges, and takes the first steps to address shortcomings and deficiencies that limit the scope of their application. This section introduces some opportunities to build on the work developed in this dissertation.

8.1.1 Acquisition Path Analysis

The metrics demonstrated in Chapter 3 were limited to considerations already raised in open literature about acquisition paths. With additional information on the technical objectives prioritized by the IAEA, new capabilities could be added to Trailmap to conduct more detailed flow analysis based on a State's facilities and technical capabilities.

8.1.2 Behaviors

The new capabilities injected into the buying and selling processes of agents allow for realistic nuclear material movement patterns to be applied throughout the fuel cycle. However, adding to the Material Buy and Sell Policies means that all new capabilities are on the agent side only. The DRE is not yet packaging-aware, leading to the potential for failed trades when partial bids are accepted, as raised in Section 4.6.6. The Material Buy and Sell Policies do not interface with each other either, they are currently independent processes.

8.1.2.1 Material Balance Areas

Because the fundamental spatial unit of international safeguards is the MBA and not the facility, Cyclus simulations for safeguards must be developed with many more agents than the same simulation designed for nuclear energy planning. These agents representing sub-facilities must be given unique composition names to prevent, for example, Reactor A1 from discharging its fuel to Reactor Z8's UNF pool, as would otherwise happen if a single set of prototypes was used to deploy all reactors.

This results in extreme inefficiency in the DRE, because most commodities in the simulation have only a single possible trading partner. This results in simulations that can take two or even three orders of magnitude longer to run due to all of the graph building, partitioning, and solving within the DRE for many graphs. Most of these graphs have only two nodes, one possible source and one possible target.

This could be addressed by formalizing the level of sub-facilty agents that bypass the DRE entirely but still record transactions. There are several possible routes of implementation. Cyclus itself could have defined trading partners. Individual agents could be designed with sub-structures that report "transactions", perhaps to a separate database table, that are technically intra-agent but include enough information to generate an inventory change on an ICR.

8.1.2.2 Packaging

Another opportunity is to build on the new capability of packaging is to develop an integrated packaging and transport unit strategy. This could be based on maximizing efficiency for the combined system rather than calculating each filling strategy only once and sequentially. The packaging strategies detailed in Section 4.6.2.1 are designed to create the fewest number of packages while maximizing the amount shipped. When transport unit restrictions are added, it is possible that a scenario arises where lowering the average package fill so as to have one more package would have resulted in a shippable number of packages based on transport unit restrictions. For example, consider the following simple scenario:

$$\begin{aligned} P^{min} &= 1 \\ P^{max} &= 2 \\ U^{min} = U^{max} &= 4 \\ I &= 6 \end{aligned}$$

Regardless of packaging fill strategy, this scenario would result in the creation of three packages of fill size two.

$$\begin{aligned} m_i &= 2 \ \forall i \in 1..3 \\ M &= \sum m_i = 6 \end{aligned}$$

Unfortunately, the transport unit restrictions do not permit three packages to be shipped, and all three trades would fail. A more integrated, iterative packaging process could return to the packaging step and identify 4 packages as a viable solution that could result in 6 units/4 packages of successful trades instead of 0 units due to trade failing.

$$m_i = 1.5 \, \forall i \in 1..4$$
$$M = \sum m_i = 6$$

This challenge has not yet arisen in practice in any of the demonstration simulations described in Chapter 7 but could limit future simulations.

8.1.3 Code 10

Many inventory KMPs from the model SSAC are not included in the Cyclus simulations. Future work could use higher-fidelity simulation agents or couple Cyclus to a processing modeling code to replicate higher-fidelity movements within MBAs. This would be especially important to do before expanding Cntaur to generate PILs, which records the snapshot inventory in an MBA by inventory KMP.

There are no shipper-receiver differences in Cntaur because Cyclus simulations are all-knowing with perfect precision of nuclear material quantities. Transactions occur once, because the material quantity is known exactly. The shipper and the receiver have the same quantity and same ID for the resource. In nuclear material accounting in the real world, shippers and receivers may each measure a transacted material and record their own mass, which may differ from each other for simple reasons of measurement, or nefarious reasons such as diversion. There is no current way to replicate this aspect of nuclear material accounting.

A next step for Cntaur would be to introduce measurement uncertainties on materials and process losses within agents. This would allow for both shipper-receiver differences at the individual inventory change level and MUF at the MBA level. This could be done on the post-processing side, as Burke *et al.* [36] and Shugart [180] have demonstrated, but a more robust solution would be to incorporate the notion of measurements within Cyclus itself.

When the two above recommendations have been implemented, Cntaur would be poised for a useful expansion to the other two types of nuclear material accounting reports, PILs and MBRs. Without more realistic intra-agent process modeling, PILs would have overly-simplified inventory KMP records, and without shipper-receiver differences or MUF, the core aspects of MBRs would be missed.

On the software side, Cntaur is not particularly memory-efficient. When first created, memory was not a priority because simulations were not large enough to strain the memory of a personal laptop. However, some of the case studies with the 10-year simulations with one-day time steps are such that the memory needed to load data at the front end of the process can strain or surpass the constraints of personal laptops. While any individual simulation can be moved to a system with more memory, there are also opportunities for improvement of memory management that would support the tool's long-term use.

8.1.4 Novel signatures of disruption

The new capabilities added to Cyclus to support one-day time step modeling and the Cntaur post-processing tool allow future users to generate synthetic nuclear material accounting reports for any fuel cycle. This work enables the ability to generate large volumes of synthetic nuclear material accounting reports from nuclear fuel cycle simulations.

The new capabilities added to Cyclus in this thesis support the ability to stochastically vary parameters between simulations across every facility. This can be used both to model benign natural variability and to replicate nefarious actions like diversion in any nuclear facility.

Future work should systematically generate many simulations based on a single nuclear fuel cycle, convert them all to Code 10 ICRs using Cntaur, and search for novel signatures of diversion or unexpected disruption, especially in other facilities than where the original action occurred.

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A CYCLUS TERMINOLOGY AND GRAMMAR

All descriptions are the author's alone. Other definitions of these terms may be found at the Cyclus website fuelcycle.org, in the fundamental concepts paper [23], in previous dissertations on Cyclus development [181, 182, 183], or in a report on Cyclus archetypes [184].

Agent An individual unit in a Cyclus simulation which is either a **region**, **institution**, or **facility**. Most agents in a simulation are facilities, which can request and/or offer a **commodity(ies)** to the **DRE**. A single agent is often used to represent a nuclear facility, an individual chemical or nuclear process, or another defined unit of space like an MBA. Agents are created from **prototypes** defined in a simulation input.

Although **regions** and **institutions** are agents, use of the term agent in this work is typically synonymous with a deployed **facility**.

API The interface between the Cyclus kernel, which manages the simulation and operates the **DRE**, and **archetypes** that contain the code needed to model individual parts of the systems.

Archetype Archetypes are a set of logic and behavior. They are the scaffolding needed to define an **agent**. They have required and optional state variables that are needed to deploy as an **agent** in a simulation. They must be compatible with the **API** in order to participate in a Cyclus simulation. Sometimes, an archetype is a wrapper around another piece of software that couples the two. Archetypes are often bundled together as a collection. For example, Cycamore is a set of archetypes that provide the basic functionality needed to model as simple fuel cycle.

DRE The dynamic resource exchange (DRE) is the multi-step market that determines the flow of nuclear **materials** and **products** at every time step in the simulation.

First, the DRE gathers information about all the requests for **resources** from every **agent** during the request for bid phase. Then, the requests are presented back to the **agents** during the RRFB stage, where each **agent** can make bids on material they would be able to provide. After the bids are submitted, the requester may place preferences on the bids, such as prioritizing a bid based on its **institution**.

Then, the DRE builds and solves graphs to determine the optimal trade for each request. Users can specify their solver in the input file. Finally, the trades are executed; the DRE goes to the winning bidder (supplier) and transacts that material to the requester.

See Matthew Gidden's dissertation at the University of Wisconsin–Madison [182] for a more detailed description.

Request (for bids) A request is the step of the **DRE** where requesting **agents** announce their interest in obtaining a certain quantity of a **commodity**, along with quality factors such as isotopic concentration or a **recipe**. This occurs at the RFB stage.

Bid A bid is an offer responding to a particular **request** for a **commodity**. The offer is to provide less than or equal to the quantity requested. The quality information, whether it matches the request exactly or not, is also provided. This occurs at the RRFB stage of the **DRE**.

An **agent** is able to make bids independently of any other bid, for example if 10 requesting **agents** each place a **request** for the supplier's full inventory, the supplier may place 10 bids, even though only one full bid or multiple partial bids adding up to the inventory will be executed. A later stage of the **DRE** determines which bids become **trades**.

Trade Trades are the final step of the DRE. Once the DRE has reconciled the requests and responding bids, a trade is the finalized agreement to transact a **commodity** between two agents.

Commodity A commodity is a description of what an **agent** requests (in-commodity) or supplies (out-commodity) to the DRE. A commodity only has a name, it has no inherent restrictions on mass, composition, or any other metric of quality. During a simulation, **resources** are designated as commodities and traded between **agents**. For example, `low_enriched_UF6` could be a commodity. An enrichment **agent** may create `low_enriched_UF6`. At a particular time step, the **agent** may create 10 kg (a quantity) of material enriched to 5% ^{235}U (a quality). Or it may create 1 kg of 1% enriched as `low_enriched_UF6`, both are designated as the same commodity by virtue of being produced by the same **agent**.

In-commodity The commodity that an **agent** requests from the DRE. An in-commodity is fixed across a **prototype**. One agent's in-commodity must match another agent's out-commodity, or their **requests** can never be fulfilled.

Out-commodity The commodity that an agent offers to the **DRE**. An out-commodity is fixed across a **prototype**. One agent's out-commodity must match another agent's in-commodity, or their **requests** can never be fulfilled.

Facility A facility is a type of **agent** that interacts with the **DRE** by requesting or offering a **commodity(ies)**. The term facility does not require that an agent include all of the processes of an actual nuclear facility. When using Cyclus for international safeguards, more than one facility agent typically comprises a nuclear facility, such as a reactor or fuel fabrication plant.

Institution All facilities must belong to an institution, and all institutions must belong to a **region**.

Library A library is a group of **archetypes**. Several simple **archetypes** are shipped with Cyclus as the Cyclus library, such as k-facility, predator, and prey. Another commonly-used library is the Cycamore library created by the Cyclus team. Referring to an **archetype** is typically formatted as `Library:Archetype`, because an **archetype** name is repeatable but combining the library and **archetype** results in a unique name.

Material Buy Policy The Material Buy Policy allows **archetypes** to engage with the **DRE** as a requester of its **in-commodity(ies)**. The buy policy acts on a single **ResBuf** and is compatible with **agent**-wide inventory limits implemented through a **total inventory tracker**.

All of the inventory management policies created in Chapters 4.3, 4.5, and 4.4 are available in the Material Buy Policy to any **archetype** developer.

Material Sell Policy

All of the packaging and transport unit capabilities created in Chapters 4.6 are available in the Material Sell Policy to any **archetype** developer.

Resource Resources are the things traded between **agents** in a simulation and tracked in the output database. Resources have two types, materials and products.

Material A material is a resource with an associated isotopic composition. It is defined by a name, a quantity, and a composition.

Product A material is a resource that may not have an isotopic composition and typically represents things that are not nuclear materials, such as people or research papers. Products are defined by a name, a quantity, and a quality.

Package A package describes minimum and/or maximum mass limitations that can be placed on a **resource** in order to have the package type applied. All **resources** in a simulation have a package type, with the default `unpackaged` type having a minimum of zero kg and a maximum of infinity.

Package types also have strategies for how to determine the fill mass of any individual packaged **resource** when being split or merged from a single (typically unpackaged type) mass.

Prototype A prototype is an **archetype** that has been given values for its parameters. For example, `Cycamore:Source` is an archetype with required parameters including `name` and `outcommod` and several optional variables including `inventory_size`. An example `Cycamore:Source` prototype defined using the XML input file style is given below. Any agents created from this prototype will have the same state variables.

```
<prototype>
    <name>Source</name>
    <Source>
        <outcommod>uranium_ore</outcommod>
        <inventory_size>100</inventory_size>
        <throughput>10</throughput>
    </Source>
</prototype>
```

Recipe A recipe defines a relative isotopic composition to be used in the simulation. Both mass and atom percentages can be used to define a recipe. Recipes are relative; they are independent of mass. The same recipe could be used to create 1 kg and 1,000 kg of 5% enriched uranium.

Region Regions are the top-level structure of a simulation. All facilities must belong to an **institution**, and all **institutions** must belong to a region. Many simulations use `agents:NullRegion`, which comes with Cyclus and exhibits no behaviors, or `Cycamore:GrowthRegion` [182] which deploys additional facility

Resource Buffer (ResBuf) Resource buffers are a **toolkit** capability that are designed to manage resources. They are implemented into the Cycamore **archetypes** and can be added to any third-party **archetype** to help manage the requesting, storage, and trading of materials. Use of the **buy policy** or **sell policy** requires at least one resource buffer.

Total inventory tracker The total inventory tracker is a capability that can manage the total inventory and space available across an arbitrary number of ResBufs. This is useful for modeling an **agent**-wide nuclear material inventory limit when **resources** are held in multiple ResBufs.

Time step Cyclus simulations are dynamic and discrete, moving and evolving through time in fixed intervals. Time steps default to 2,629,846 seconds or approximately one average month, but may be specified by the user in an input file. Time steps for any individual simulation are fixed.

International safeguards typically requires precision of nuclear material movements on the day level, so most simulations in this work are one day long, or 86,400 seconds. The fundamental unit of time in Cyclus is the second.

Toolkit The toolkit is a set of capabilities that can be added into **archetypes** to help with managing aspects of their models outside the core technical capabilities. For example, toolkit snippets are available to structure **archetypes** as **commodity** producers, to manage resources in **ResBufs** and **total inventory trackers**, and to engage with the **DRE** through a **buy policy** or **sell policy**.

archetype developers often prioritize and have the most experience in developing the scientific aspects of their model(s), and many of the toolkit items allow them to focus on implementing those technical aspects rather than spending their time learning how to interface with the CYCLUS internals.

B.1 States

The IAEA refers to nations as States, traditionally capitalized. The same style is used for both real and fictitious countries used in this dissertation.

B.2 Nuclear material accounting

A facility's accounting structures and measurement plan are sometimes referred to as MC&A, or nuclear material accountancy and control (NMAC), especially when the focus includes nuclear security and, or instead of international safeguards. MC&A is a term compatible with domestic safeguards in the United States and is used by the NRC and DOE. The IAEA does not use the acronyms MC&A or NMAC in the context of international safeguards, instead referencing nuclear material accounting as a portion of a SSAC.

The *Nuclear Material Accounting Handbook* [185] says, "The SSAC shall be based on **a structure of material balance areas (MBAs)** and shall provide for the establishment of a measurement system, a records and reports system, procedures for taking a physical inventory and provisions to ensure that accounting procedures and arrangements are correctly operated", emphasis added.

While a small number of IAEA publications have shortened nuclear material accounting as NMA, the *Nuclear Material Accounting Handbook* and other high-level safeguards publications do not.

This work follows IAEA terminology and will refer to a SSAC when discussing an entire State and nuclear material accounting system or structure when discussing individual facilities or LOFs. In some cases, accounting is managed at the region and not the State level. Countries in the European Union (EU) all participate in Euratom and have a regional system of accounting for and control of nuclear material (RSAC) [186, 187]. This work assumes all States have independent SSACs.

B.3 Safeguards conclusions

For States with a CSA and an Additional Protocol in force

The IAEA draws safeguards conclusions for each State each year and shares them publically through their Annual Report [188]. In 2023, the IAEA evaluated 136 States with both CSAs and APs in force. In 2023, 74 States were given the first conclusion, 62 the second, and none the third.

1. If the IAEA's Secretariat has completed all evaluations and found no indication of the diversion of declared nuclear material from peaceful nuclear activities, no indication of undeclared production or processing of nuclear material at declared facilities and locations outside facilities, and no indication of undeclared nuclear material or activities, the Secretariat can conclude, on this basis, that all nuclear material remained in peaceful activities; and
2. If the IAEA's Secretariat found no indication of the diversion of declared nuclear material from peaceful nuclear activities, and no indication of undeclared production or processing of nuclear material at declared facilities and locations outside facilities, but evaluations regarding the absence of undeclared nuclear material and activities remained ongoing, the Secretariat can conclude, on this basis, that declared nuclear material remained in peaceful activities.
3. The IAEA Secretariat cannot draw any safeguards conclusions.

For States with a comprehensive safeguards agreement (CSA) but without an Additional Protocol in force

There were 45 States with CSAs in force but no AP in force. All States in this category were given the first conclusion.

1. If the IAEA's Secretariat found no indication of the diversion of declared nuclear material from peaceful nuclear activities, and no indication of undeclared production or processing of nuclear material at declared facilities and locations outside facilities, the Secretariat can conclude, on this basis, that declared nuclear material remained in peaceful activities.
2. The IAEA Secretariat cannot draw any safeguards conclusions.

Under item-specific safeguards agreements

Three States have safeguards agreements based on INFCIRC/66/Rev.2 in force. All are non-signatories of the NPT. They were all given the first conclusion.

1. If the IAEA's Secretariat found no indication of the diversion of nuclear material or of misuse of the facilities or other items to which safeguards had been applied, the Secretariat can conclude, on this basis, that nuclear material, facilities or other items to which safeguards had been applied remained in peaceful activities.
2. The IAEA Secretariat cannot draw any safeguards conclusions.

For States with voluntary offer safeguards agreements

5 States have both VOAs and APs in force, the nuclear-weapon States. The United States of America, the United Kingdom of Great Britain and Northern Ireland, France, the Russian Federation, and the People's Republic of China were all given the first conclusion.

1. If the IAEA's Secretariat found no indication of the undeclared withdrawal from safeguards of nuclear material to which safeguards had been applied, the Secretariat can conclude, on this basis, that nuclear material in selected facilities to which safeguards had been applied remained in peaceful activities or had been withdrawn from safeguards as provided for in the agreements.
2. The IAEA Secretariat cannot draw any safeguards conclusions.

For States with no safeguards agreements in force

No safeguards conclusions were drawn for the remaining four States Party to the NPT without CSAs in force.

1. The IAEA Secretariat cannot draw any safeguards conclusions.

Finally, the IAEA did not implement safeguards on the Democratic People's Republic of Korea (DPRK) and could not draw any conclusion.

Declaring packages

Similar to recipes, packages are declared as an optional, repeatable block in a Cyclus input file. Archetypes that use packages must pull from the simulation-wide list of packages, they should not be declared directly in an prototype (facility) block. An example package definition is shown in Listing C.1.

```xml
<package>
    <name>PackageExample</name>
    <fill_min>2.5</fill_min>
    <fill_max>3</fill_max>
    <strategy>equal</strategy>
</package>
```

Listing C.1: Package type declaration

Resource buffers are widely used for inventory management in Cycamore, the NFC facility agents created and maintained by the Cyclus team, as well as other third-party agents. The default behavior of resource buffers is to convert all resources to the `unpackaged` package upon entry; by default the buffer considers all resources to be completely mutable.

In certain cases retaining packaging information upon entry into a resource buffer is useful however, especially where resources represent immutable objects that should not have their quantity or packaging type changed upon entry or exit of the buffer.

Transport units are declared similarly to packages. An example is shown in Listing C.2.

```xml
<transportunit>
    <name>TransportUnitExample</name>
    <fill_min>3</fill_min>
    <fill_max>5</fill_max>
    <strategy>hybrid</strategy>
</transportunit>
```

Listing C.2: Transport unit declaration

C.1 Case studies

Each of the reactor systems used in the case studies was developed from model reactors or reactors used in options developed for the Fuel Cycle Options Catalog [130]. Each of the options includes isotopic information from a linked FCDP. In some cases, the isotopic information used to develop Cyclus recipes for used and recycled nuclear fuels was given a different title than the general option title. To avoid any

Table C.1: Fuel Cycle Options Catalog titles for once-through and limited recycle case studies

Case	Type	Name
1	Model Reactor	Westinghouse AP1000
2	Model Reactor	AtkinsRéalis CANDU 6
3	Model Reactor	HTR-PM
4	Model Reactor	SPR
5	Option Title	Sodium-Cooled Fast Reactor (Breed and Burn) using Natural Uranium Fuel with no Recycling
	FCDP Title	Breed and Burn SFR without Separation
6	Option Title	Sodium-Cooled Fast Reactor (Breed and Burn) using Natural Uranium Fuel with limited recycling
	FCDP Title	SFR B&B with Fuel Reconditioning
7	Option Title	Pressurized Water Reactor using Low-Enriched Uranium Fuel; Accelerator Driven System using Plutonium Fuel
	FCDP Title	Recover Pu from PWR and Burn in ADS
8	Option Title	Pressurized Water Reactor using Low-Enriched Uranium Fuel (SMR)
	FCDP Title	SMR-uranium oxide (UOX) to discharged fuel (DF)

confusion, Table C.1 and Table C.2 give the full name for the model reactor, or the Fuel Cycle Options Catalog title and the FCDP title.

Table C.2: Fuel Cycle Options Catalog titles for continuous recycle case studies

Case	Type	Name
9	Option Title	Sodium-Cooled Fast Reactor using Plutonium, Natural Uranium, and Recovered Uranium Fuel
	FCDP Title	Sodium-Cooled Fast Reactor using Plutonium, Natural Uranium, and Recovered Uranium Fuel
10	Option Title	Reduced-Moderation Boiling Water Intermediate Reactor Recycling Transuranics
	FCDP Title	Self-sustainable RBWR with an intermediate spectrum
11	Option Title	Sodium-Cooled Fast Reactor using Transuranic and Uranium Fuel; Pressurized Water Reactor using Transuranic and Uranium Fuel
	FCDP Title	SFR(TRU/U) to PWR(TRU/U) for Full Recycling
12	Option Title	Pressurized Water Reactor using Low-Enriched Uranium Fuel; PWR using Plutonium and Recovered Uranium Fuel
	FCDP Title	Pressurized Water Reactor using Low-Enriched Uranium Fuel; PWR using Plutonium and Recovered Uranium Fuel
13	Option Title	Molten Salt Reactor using Thorium, Uranium-233, and Transuranic Fuel
	FCDP Title	U-233 Recycle in MSR

C.1.1 Power reactors

Power reactors were developed with a generic structure, shown in Figure C.1. All power plant facilities are a single MBA. Each reactor has its own fresh fuel vault agent and reactor agent. Depending on the case, each reactor may have its own UNF pool for immediate wet storage after reactor discharge or may share a storage pool with one or more other reactors. Each power plant has only a single shipper agent that sends MPCs or other transport containers of UNF for recycling or consolidated dry storage.

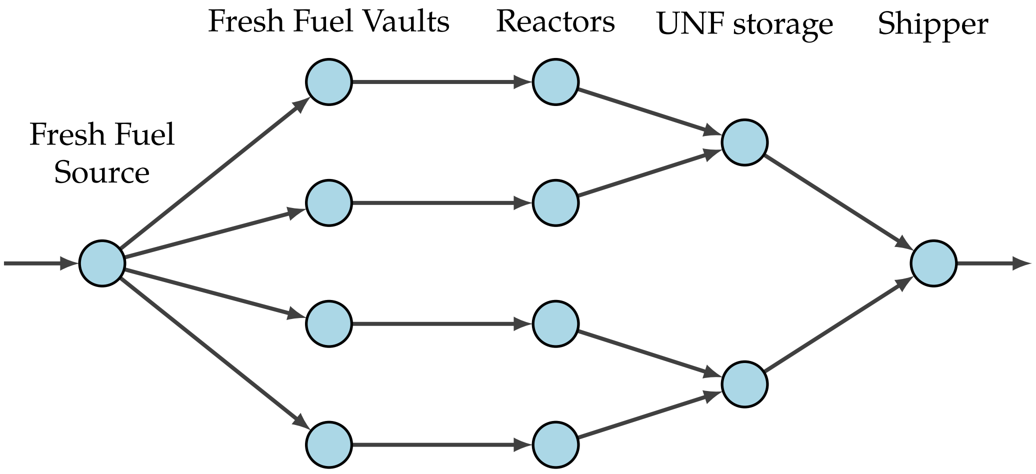

Figure C.1: Each reactor in a power plant has its own fresh fuel vault. Several reactors may share a UNF pool or storage facility. There is only one shipper agent.

C.1.2 Back end

The case studies in this work use the `Cycamore:Reactor` archetype. This is the simplest reactor model developed for Cyclus static compositional transformations. UNF compositions were developed from the related FCDP or other published results. Some compositions may be reported after a cooling period.

All thorium, uranium, plutonium, and MA nuclides will be included in the UNF if they have a weight fraction above 1e-6, as well as at least 10 fission products.

C.1.3 Packaging and Transportation

Packages and transport units were developed to replicate real nuclear material packaging strategies when available. When a relevant model nuclear material package was not available, surrogate packages were developed from physically meaningful quantities. For example, no facility currently produces and ships mixed-actinide oxide, including RU, recycled thorium, and TRU in commercial quantities. Because no package exists for commercial-scale quantities of this material, the simulation package was set at 300 kg, or approximately the mass of material used to form one recycled BWR fuel assembly, the type used in Case 10, when mixed with a makeup fertile fuel.

C.2 Code 10

These appendices were approved as part of *Advanced Algorithms for Scrutiny of Mandatory State Reports Declarations to the IAEA: Final Project Report*, LA-UR-24-24919

C.2.1 Code 10 labels not implemented in CNTAUR

Table C.3: Weight elements not implemented in CNTAUR

Label	Name	Unit
600	Unified uranium	grams
650	U-234 isotopic content	grams
680	U-236 isotopic content	grams
690	U-238 isotopic content	grams
710	Pu-238 isotopic content	grams
720	Pu-239 isotopic content	grams
730	Pu-240 isotopic content	grams
740	Pu-241 isotopic content	grams
750	Pu-242 isotopic content	grams
760	Pu-239 + Pu-241 isotopic content	grams
770	Natural uranium fissile content	grams
780	Depleted uranium fissile content	grams

Table C.4: Data elements not implemented in Cntaur

Label	Name	Description
099	Concise Note Reference	Provides the country, facility, MBA, report as a whole or entry to which the Concise Note refers
310	State Accounting System Record Identification	Identifies the corresponding information in the State accounting system
390	Concise Note Indicator	Calls attention to a Concise Note attached
391	Text of Concise Note	Other unformatted information
436	Operator's Material Description Code	The code used by the operator to identify the type of nuclear material
445	Non-Latin Alphabet Identification	A code to indicate that a non-Latin alphabet was used in the report and to identify that alphabet
447	Shipper's Batch Name	Identifies the shipper's batch name in the reporting of a receipt

C.2.2 CNTAUR Code 10 Demonstration

A minimal working example of CNTAUR is presented in this Appendix. The country in question is fictitious country AA, with single reactor facility AA01. The reactor's parameters have been simplified to demonstrate the capability of CNTAUR.

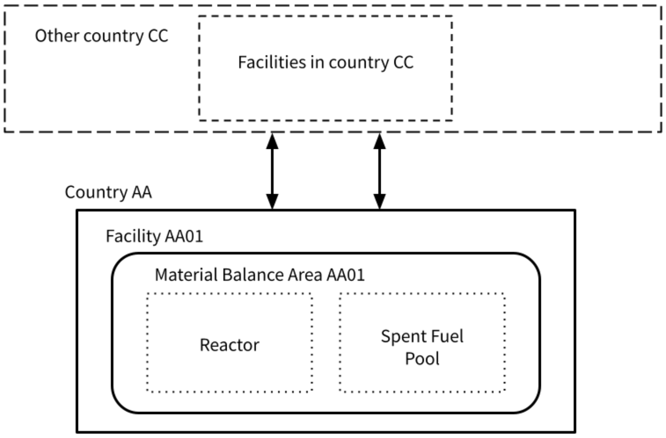

Figure C.2: Accounting structure of example state AA

Input files

CYCLUS input file

```
<simulation>
<control>
    <dt>86400</dt>
    <duration>121</duration>
    <startyear>2020</startyear>
    <startmonth>1</startmonth>
</control>

<archetypes>
    <spec><lib>agents</lib><name>NullRegion</name></spec>
    <spec><lib>agents</lib><name>NullInst</name></spec>
    <spec><lib>cycamore</lib><name>Source</name></spec>
    <spec><lib>cycamore</lib><name>Reactor</name></spec>
    <spec><lib>cycamore</lib><name>Sink</name></spec>
    <spec><lib>cycamore</lib><name>Storage</name></spec>
</archetypes>

<facility>
    <name>Source</name>
```

```
        <config>
            <Source>
                <outcommod>fuel</outcommod>
                <outrecipe>fuel_recipe</outrecipe>
            </Source>
        </config>
    </facility>

    <facility>
        <name>Reactor</name>
        <config>
            <Reactor>
                <fuel_incommods>
                    <val>fuel</val>
                </fuel_incommods>
                <fuel_inrecipes>
                    <val>fuel_recipe</val>
                </fuel_inrecipes>
                <fuel_outcommods>
                    <val>spent_fuel</val>
                </fuel_outcommods>
                <fuel_outrecipes>
                    <val>spent_fuel_recipe</val>
                </fuel_outrecipes>
                <assem_size>100</assem_size>
                <cycle_time>30</cycle_time>
                <n_assem_core>3</n_assem_core>
                <n_assem_batch>1</n_assem_batch>
            </Reactor>
        </config>
    </facility>

    <facility>
        <name>SpentFuelPool</name>
        <config>
            <Storage>
                <in_commods>
                    <val>spent_fuel</val>
                </in_commods>
                <out_commods>
                    <val>spent_fuel_cooled</val>
                </out_commods>
                <residence_time>14</residence_time>
            </Storage>
        </config>
```

```xml
    </facility>

    <facility>
        <name>Sink</name>
        <config>
            <Sink>
                <in_commods>
                    <val>spent_fuel_cooled</val>
                </in_commods>
            </Sink>
        </config>
    </facility>

    <recipe>
        <name>fuel_recipe</name>
        <basis>mass</basis>
        <nuclide>
            <id>922350000</id>
            <comp>0.0265</comp>
        </nuclide>
        <nuclide>
            <id>922380000</id>
            <comp>0.8442</comp>
        </nuclide>
        <nuclide>
            <id>80160000</id>
            <comp>0.1186</comp>
        </nuclide>
    </recipe>

    <recipe>
        <name>spent_fuel_recipe</name>
        <basis>mass</basis>
        <nuclide><id>922340000</id><comp>0.00012</comp></nuclide>
        <nuclide><id>922350000</id><comp>0.00456</comp></nuclide>
        <nuclide><id>922360000</id><comp>0.00311</comp></nuclide>
        <nuclide><id>922380000</id><comp>0.73401</comp></nuclide>
        <nuclide><id>942380000</id><comp>0.00017</comp></nuclide>
        <nuclide><id>942390000</id><comp>0.00384</comp></nuclide>
        <nuclide><id>942400000</id><comp>0.00197</comp></nuclide>
        <nuclide><id>942410000</id><comp>0.00080</comp></nuclide>
        <nuclide><id>942420000</id><comp>0.00051</comp></nuclide>
        <nuclide><id>80160000</id><comp>0.11852</comp></nuclide>
        <nuclide><id>10010000</id><comp>0.13239</comp></nuclide>
    </recipe>
```

```

    <region>
        <name>SingleRegion</name>
        <config>
            <NullRegion/>
        </config>
        <institution>
            <name>SingleInstitution</name>
            <config>
                <NullInst/>
            </config>
            <initialfacilitylist>
                <entry><prototype>Source</prototype><number>1</number></
                    entry>
                <entry><prototype>Reactor</prototype><number>1</number></
                    entry>
                <entry><prototype>SpentFuelPool</prototype><number>1</
                    number></entry>
                <entry><prototype>Sink</prototype><number>1</number></
                    entry>
            </initialfacilitylist>
        </institution>
    </region>

</simulation>
```

Country file

Listing C.3 shows an MBA file for a simplified reactor model containing only a `Cycamore:Reactor` and a `Cycamore:Storage` representing an UNF storage pool. This MBA file is the same one shown in Section 5.2.3.

```
    <MBA>
        <name>AA01</name>
        <country>AA</country>
        <facility>AA01</facility>
        <agents>
            <agent>Reactor_Id15</agent>
            <agent>SpentFuelPool_Id16</agent>
        </agents>
        <reactor_agent>
            <agent>Reactor_Id15</agent>
        </reactor_agent>
        <inventory_KMPs>
```

```
            <KMP>
                <name>B</name>
                <agent>Reactor_Id15</agent>
            </KMP>
            <KMP>
                <name>C</name>
                <agent>SpentFuelPool_Id16</agent>
            </KMP>
        </inventory_KMPs>
        <flow_KMPs>
            <in>
                <KMP>
                    <name>1</name>
                    <MBA>else</MBA>
                </KMP>
            </in>
            <out>
                <KMP>
                    <name>2</name>
                    <MBA>else</MBA>
                </KMP>
            </out>
        </flow_KMPs>
        <generate_reports>True</generate_reports>
    </MBA>
```

Listing C.3: MBA file snippet for a reactor with one MBA (AA01)

Material description code file

The three types of nuclear materials in this simulation include fresh nuclear fuel, imported from another country, spent fuel discharged from the reactor, and spent fuel "cooled" and ready to ship to another facility (in this simulation, to a fuel take-back out of country).

```
{
    "fuel": "B/Q/2/F",
    "spent_fuel": "B/Q/1/G",
    "spent_fuel_cooled": "B/Q/3/G"
}
```

Listing C.4: MDC file snippet linking commodities and material descriptions

CNTAUR Output

The following Code 10 reports were produced

```
001:OI/AA;1#002:1/6#003:20200302#006:TEST,TEST#010:I#015:20200101/20200131#207:AA01#307:AA01#309:N#370:CC/CC#372:AA/AA01#407:1#411:RF#412:20200101#430:B/Q/2/F#436:fuel#446:13#447:13#469:N#470:1#630:88011.7G#670:2678.7G#
001:OI/AA;1#002:2/6#003:20200302#006:TEST,TEST#010:I#015:20200101/20200131#207:AA01#307:AA01#309:N#310:1#370:CC/CC#372:AA/AA01#407:1#411:RF#412:20200101#430:B/Q/2/F#436:fuel#446:15#447:15#469:N#470:1#630:88011.7G#670:2678.7G#
001:OI/AA;1#002:3/6#003:20200302#006:TEST,TEST#010:I#015:20200101/20200131#207:AA01#307:AA01#309:N#310:2#370:CC/CC#372:AA/AA01#407:1#411:RF#412:20200101#430:B/Q/2/F#436:fuel#446:17#447:17#469:N#470:1#630:88011.7G#670:2678.7G#
001:OI/AA;1#002:4/6#003:20200302#006:TEST,TEST#010:I#015:20200101/20200131#207:AA01#307:AA01#309:N#310:4#370:AA/AA01#372:AA/AA01#407:A#411:LN#412:20200131#430:B/Q/1/G#436:spent_fuel#446:76#447:76#469:N#470:1#630:13831.7G#670:2222.7G#
001:OI/AA;1#002:5/6#003:20200302#006:TEST,TEST#010:I#015:20200101/20200131#207:AA01#307:AA01#309:N#310:3#370:CC/CC#372:AA/AA01#407:1#411:RF#412:20200131#430:B/Q/2/F#436:fuel#446:83#447:83#469:N#470:1#630:88011.7G#670:2678.7G#
001:OI/AA;1#002:6/6#003:20200302#006:TEST,TEST#010:I#015:20200101/20200131#207:AA01#307:AA01#309:N#310:4#370:AA/AA01#372:AA/AA01#407:A#411:NP#412:20200131#430:B/Q/1/G#436:spent_fuel#446:76#447:76#469:N#470:1#700:729.0G#
```

```
001:OI/AA;2#002:1/1#003:20200330#006:TEST,TEST#010:I#015:20200201/20200228#207:AA01#307:AA01#309:N#310:5#370:AA/AA01#372:CC/CC#407:2#411:SF#412:20200215#430:B/Q/3/G#436:spent_fuel_cooled#446:76#447:76#469:N#470:1#620:74.18K#700:729.0G#
```

```
001:OI/AA;3#002:1/4#003:20200430#006:TEST,TEST#010:I#015:20200301/20200331#207:AA01#307:AA01#309:N#310:7#370:AA/AA01#372:AA/AA01#407:A#411:LN#412:20200303#430:B/Q/1/G#436:spent_fuel#446:145#447:145#469:N#470:1#630:13831.7G#670:2222.7G#
001:OI/AA;3#002:2/4#003:20200430#006:TEST,TEST#010:I#015:20200301/20200331#207:AA01#307:AA01#309:N#310:6#370:CC/CC#372:AA/AA01#407:1#411:RF#412:20200303#430:B/Q/2/F#436:fuel#446:152#447:152#469:N#470:1#630:88011.7G#670:2678.7G#
001:OI/AA;3#002:3/4#003:20200430#006:TEST,TEST#010:I#015:20200301/20200331#207:AA01#307:AA01#309:N#310:7#370:AA/AA01#372:AA/AA01#407:A#411:NP#412:20200303#430:B/Q/1/G#436:spent_fuel#446:145#447:145#469:N#470:1#700:729.0G#
001:OI/AA;3#002:4/4#003:20200430#006:TEST,TEST#010:I#015:20200301/20200331#207:AA01#307:AA01#309:N#310:8#370:AA/AA01#372:CC/CC#407:2#411:SF#412:20200318#430:B/Q/3/G#436:spent_fuel_cooled#446:145#447:145#469:N#470:1#620:74.18K#700:729.0G#
```

```
001:OI/AA;4#002:1/4#003:20200530#006:TEST,TEST#010:I#015:20200401/20200430#207:
    AA01#307:AA01#309:N#310:10#370:AA/AA01#372:AA/AA01#407:A#411:LN
    #412:20200403#430:B/Q/1/G#436:spent_fuel#446:214#447:214#469:N
    #470:1#630:13831.7G#670:2222.7G#
001:OI/AA;4#002:2/4#003:20200530#006:TEST,TEST#010:I#015:20200401/20200430#207:
    AA01#307:AA01#309:N#310:9#370:CC/CC#372:AA/AA01#407:1#411:RF#412:20200403#430:
    B/Q/2/F#436:fuel#446:221#447:221#469:N#470:1#630:88011.7G#670:2678.7G#
001:OI/AA;4#002:3/4#003:20200530#006:TEST,TEST#010:I#015:20200401/20200430#207:
    AA01#307:AA01#309:N#310:10#370:AA/AA01#372:AA/AA01#407:A#411:NP
    #412:20200403#430:B/Q/1/G#436:spent_fuel#446:214#447:214#469:N#470:1#700:729.0
    G#
001:OI/AA;4#002:4/4#003:20200530#006:TEST,TEST#010:I#015:20200401/20200430#207:
    AA01#307:AA01#309:N#310:11#370:AA/AA01#372:CC/CC#407:2#411:SF#412:20200418#430:
    B/Q/3/G#436:spent_fuel_cooled#446:214#447:214#469:N#470:1#620:74.18K#700:729.0
    G#
```

QCVS configuration

In order to verify the working example above using QCVS, the tool was configured with the data of the the fictional countries. Because country AA is not required to know the facility and MBA codes of their trading partner country CC, those were left blank.

Table C.5: Configuration of QCVS

File	Data
Countries	AA, CC
DomesticFac	AA01
DomesticMBA	AA01
ForeignFac	
ForeignMBA	

The reports above passed the QCVS quality control checks.