

# Modeling Material Diversion with the Cyclus Nuclear Fuel Cycle Simulator

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## Abstract

Already the dominant source of clean energy, nuclear power is growing at a rapid pace. While beneficial to a world confronting climate change, there are increasingly serious nuclear security and non-proliferation concerns attendant to this expansion. As a result, it is imperative to develop credible methods to verify compliance with treaties that control fissile material production, such as the Nuclear Nonproliferation Treaty (NPT) or a potential Fissile Material Cutoff Treaty (FMCT). As part of the Consortium for Verification Technology, the Cyclus fuel cycle simulator is being used to model current and next-generation nuclear fuel cycles and inform treaty verification. Cyclus is an agent-based, systems-level simulator that tracks discrete material flow through the entire fuel cycle, from mining through burnup in reactors to a repository, or alternatively through one or more iterations of reprocessing. Cyclus includes socio-behavior models of individual actors, facilitating the study of clandestine material diversion from declared fuel cycles. Cyclus also features a region-institution-facility hierarchy that can incorporate the effects of tariffs and sanctions in a regional or global context. This paper presents initial Cyclus simulations of highly enriched uranium diversion from a declared once-through fuel cycle. Simulated material flow signals are analyzed to look for potential diversion of nuclear material for nuclear weaponry use.

## 1 Introduction

Nuclear expertise is rapidly expanding around the world as demand for energy increases steadily. Because nuclear energy is clean and carbon-neutral, climate change concerns further tilt the scales making nuclear power appealing to a growing number of countries [1]. China is already investing heavily in nuclear power, planning to triple its generating capacity from 19 gigawatt electrical (GWe) to 58 GWe by 2020 [2]. As climate change becomes increasingly important with respect to national security, the perception of the risk inherent to nuclear energy is decreasing and states are embracing nuclear energy as a reliable large-scale source of carbon-neutral energy. However, the expansion of nuclear power amplifies nuclear security concerns, because the same technologies used to produce nuclear fuel can also be exploited in the pursuit of nuclear weapons. Moreover, in the 70 years since nuclear bombs were dropped on Hiroshima and Nagasaki, the knowledge and technology required to make these weapons has proliferated around the globe [3]. There are now nine states that have developed their own nuclear weapons either through indigenous research or transfer of knowledge from existing programs. As nuclear power becomes more ubiquitous, it becomes ever

more important to meaningfully decouple the nuclear expertise required for the pursuit of energy from that of nuclear weapons.

## 1.1 Sensitive Parts of the Nuclear Fuel Cycle

Two nuclear technologies are of particular concern for proliferation, uranium enrichment and plutonium reprocessing. Uranium enrichment is required for the once-through fuel cycles that are dominant around the world today, and used exclusively in the United States (US). A once-through fuel cycle includes a source of natural uranium such as a mine, and is comprised primarily of non-fissile 99.3%  $^{238}\text{U}$ , with only 0.7% fissile  $^{235}\text{U}$  that is able to undergo nuclear fission. Concentrations of 3-5% fissile  $^{235}\text{U}$  are typical for fueling a nuclear power reactor. (Research reactors use higher levels of enrichment and there are ongoing efforts to phase out those that use enrichments above 20%). Enrichment facilities are used to increase the concentration of  $^{235}\text{U}$  from natural stock to the desired amount. Fuel is then burned in a nuclear reactor and the remaining material, which includes the majority of the original  $^{238}\text{U}$ , short- and long-lived fission products, and  $\sim 1\%$  Pu ( $^{239}$  and  $^{240}$ ), is then stored as waste. The enrichment phase of the fuel cycle is a proliferation concern because in principle it can be used to increase the concentration of  $^{235}\text{U}$  up to the 90% or more typically used to make a nuclear weapon [4].

Plutonium reprocessing is a proliferation concern because the technique can be used either to make recycled fuel or to make weapons-grade fissile material. Several countries are developing nuclear reactors that can accommodate recycled fuel, providing the possibility of a closed fuel cycle in which the burning of nuclear fuel would at the same time generate new nuclear fuel [5]. Recycled fuel is plutonium-based rather than uranium-based, and is made by separating the components of spent uranium fuel to extract the plutonium concentrations of fissile  $^{239}\text{Pu}$ . This material can then be blended with uranium to make mixed oxide (MOX) fuel. (MOX can also be made by sourcing the plutonium from decommissioned weapons). The concentration of  $^{239}\text{Pu}$  depends on the amount of time the fuel was burned in the reactor, and can be upwards of 50%. Specially designed irradiation of uranium fuel can produce a plutonium component with  $^{239}\text{Pu}$  concentrations up to 93%, known as weapons-grade plutonium (WGP). Reprocessing has been considered in the US at several times over the past half-century. However, a host of political, economic, environmental and strategic concerns have pushed the issue of reprocessing out of the technical realm and it has become a contentious political topic, currently the US is pursuing only basic science research in this field [6, 7].

## 1.2 Use of Treaties to Curtail Proliferation

While it has not proven possible to prevent the spread of nuclear knowledge entirely, international treaties have been used in an attempt to minimize it. The NPT, which has been signed by 190 states including the original five nuclear weapons states, has codified a set of rules and norms for allowing the peaceful pursuit of nuclear energy [8]. The NPT created the International Atomic Energy Agency (IAEA), whose role is to verify compliance with the treaty by periodically inspecting facilities related to nuclear technology. Other relevant treaties include Comprehensive Nuclear-Test-Ban Treaty (CTBT), which placed a moratorium on testing nuclear weapons, and the Strategic Arms Reduction Treaties (START) in which the US and Russia agreed to nuclear arms reductions [9, 10]. (The CTBT has been signed by 164 states but has not yet entered into force).

These treaties have done much to prevent the spread of nuclear weapons knowledge, but they do not address the weapons production capabilities of states that already possess nuclear weapons.

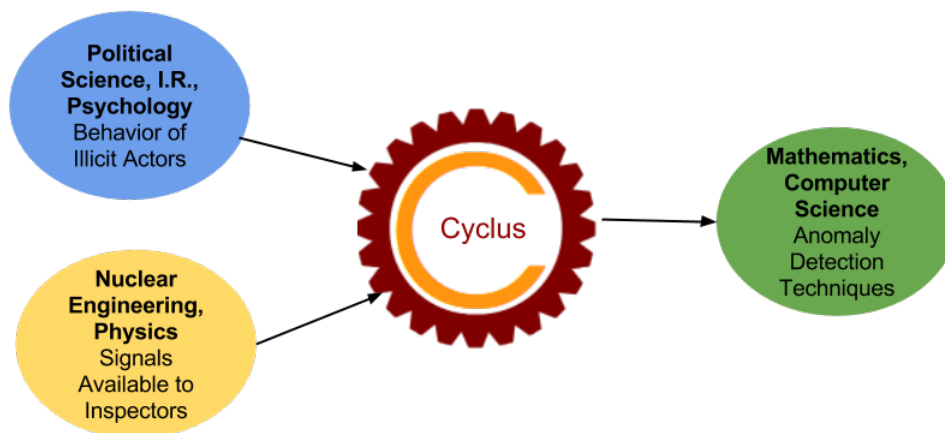


Fig. 1: The CYCLUS nuclear fuel cycle simulator provides a testbed to integrate innovations in treaty verification across many disciplines.

A potential FMCT would place limits on the amount of weapons-grade fissile material that each signatory state could stockpile, possibly including current stockpiles in the case of weapons states. However, a major unresolved issue is the difficulty of developing verification techniques to ensure compliance [11]. Furthermore, measuring nuclear material for treaty verification is itself a sensitive issue, as even collecting the spectra of a material to confirm its authenticity can potentially expose sensitive information to the inspecting party [12]. Particularly if non-weapon states are to contribute to treaty verification, it is important to prevent the further dissemination of nuclear weapons knowledge.

An effective treaty verification regime must synthesize knowledge from the realms of political science, international relations, nuclear physics and engineering, and even behavioral psychology. Figure 1 illustrates the role of a fuel cycle simulator such as CYCLUS in bringing together these disparate fields to provide insights into proposed verification technologies. A fuel cycle simulator tracks the flow of nuclear material through the facilities in a fuel cycle. It creates synthetic data, such as what would be available to an inspector, for many different facilities simultaneously while incorporating a system-level perspective of proliferation scenarios. This synthetic data can then be used as a testbed to investigate the efficacy of new detection and analysis techniques. In this way, simulators can be used to to illucidate the strengths and weaknesses of various verification strategies.

## 2 The Cyclus Fuel Cycle Simulator

The Computational Nuclear Engineering Research Group (CNERG)<sup>1</sup> group at the University of Wisconsin has developed the CYCLUS<sup>2</sup> nuclear fuel cycle simulator to model all aspects of the nuclear fuel cycle in a flexible way [13, 14, 15]. CYCLUS produces a database file containing information on the flow of nuclear material through the fuel cycle at each timestep. The database provides information on facility inventories, material composition, transactions between facilities, and facility

<sup>1</sup> <http://cnerg.github.io/>

<sup>2</sup> <http://fuelcycle.org/>

build and decommissioning histories, among others.

CYCLUS is designed using an agent-based framework, meaning that each actor in a fuel cycle (such as a mine, a nuclear reactor, or even a governing body) is modeled as an independent agent [16, 17]. Each agent in the simulation is self-contained and may include physics, economics, or behavioral components [18, 19, 20]. The agents interact with one another through the dynamic resource exchange (DRE), which facilitates the trading of resources and commodities [21]. At each timestep, agents can choose to request resources. Resources are defined using both a quantity (e.g. 1 metric ton), and a quality, such as having a composition of 99.7%  $^{238}\text{U}$  and 0.3%  $^{235}\text{U}$ . The DRE then solicits bids from any facilities that are interested in offering those resources. Resources can be offered as bids even if they do not exactly match the requested material. For example, a reactor might request a commodity called “fuel”, which it has defined as being uranium oxide (UOX). It may receive two bids for “fuel” that are specified as UOX and MOX, having two distinct isotopic compositions. After the bids are received, the requestor is able to state a preference for one bid over another. Finally, once the preferences have been applied, the DRE calculates all potential trades across all agents, then executes an optimization algorithm to find the solution that most closely fulfills a maximum of requests. It is possible that as a result of the preference adjustment, no trades are executed for some facilities in a given time step. Once this solution is found, material is transferred across the facilities and the timestep is concluded.

Although CYCLUS was designed to assess the transition from once-through fuel cycles to alternative next-generation scenarios including technologies such as spent fuel recycling, it is also an excellent tool for examining proliferation issues. Other fuel cycle simulators designed to study energy issues are typically too inflexible to be used for other purposes. For example, they may have extremely accurate physics models of reactor burnup, but no ability to vary or modify other facilities in the fuel cycle. CYCLUS has three key features that make it well-suited to non-proliferation studies: it is *agent-based*, it incorporates *social and behavioral interaction models*, and it tracks *discrete materials*.

## 2.1 Agent-Based

Agent-based design is important in studying non-proliferation because it allows the comparison of different scenarios by changing just one aspect of the simulation at a time. CYCLUS features a modular design in which individual facility models can be swapped in otherwise identical fuel cycles for comparison. For example, a user could compare enrichment technologies by creating two different enrichment modules, one using gaseous diffusion and the other using centrifuge technology. Then two simulations can be run where the entire fuel cycle is identical except for the two different enrichment designs, and the results can therefore be directly compared. The other benefit of the agent-based model is that simulations can be made as detailed facility models, generalized systems-level models, or a hybrid of both. This facilitates the studying of how changes in one part of the system will impact other areas. In proliferation studies, this means that the effects on all other facilities from diversion at a single site can be modeled simultaneously.

## 2.2 Behavioral Modeling

The preference adjustment phase of the DRE allows for the introduction of interaction behaviors. Behavioral modeling is critical to studying non-proliferation because it can be used to approximate real-world motivations and interactions that are not captured by economics or other conventional

decision-making models. Each agent can prioritize bids for resources in any way it chooses. A specific agent might have preferences based on material composition, physical proximity between facilities, or allowed and disallowed trading partners, which are implemented in a region-institution-facility hierarchy that enables economic modeling [22]. Individual facilities can be managed by institutions, such as multinational corporations, utilities, government agencies, etc. Facilities and institutions can then be ascribed to distinct regions, which may represent geographical regions, political alliances or economic trading partners. This feature allows CYCLUS to model tariffs, sanctions and other types of economic agreements. Agents may also make decisions about interacting at each timestep based on their own internal logic, for example, an illicit facility may choose not to trade at every timestep in an attempt to avoid detection.

## 2.3 Discrete Materials

CYCLUS tracks discrete material flow through the simulation, meaning that once a material enters the simulation, its location and quality is tracked at all remaining timepoints [23]. Discrete material modeling is useful in studying non-proliferation because material found anywhere in the fuel cycle can be tracked back to its source, providing attribution for illicit behavior. CYCLUS includes nuclear data from PyNE,<sup>3</sup> a computational nuclear science tool that enables calculation of decay and transmutation [24]. As a result, CYCLUS can model decay of materials and track all decay products from a parent isotope, facilitating studies of heat loading, radiation exposure, and other derived fuel cycle metrics [25]. This also opens the door to using CYCLUS to model historical events, with applications in nuclear forensics and archeology.

## 3 A Diversion Scenario: Highly Enriched Uranium

As a part of the Consortium for Verification Technology (CVT)<sup>4</sup>, CYCLUS is being used to incorporate socio-behavioral modeling into simulations of highly enriched uranium (HEU) diversion from a declared fuel cycle with the goal of improving detection techniques. In the simplest implementation, material is diverted from the enrichment facility. Figure 2 illustrates a toy model of this portion of the fuel cycle. A facility such as a mine supplies natural uranium (0.7% <sup>235</sup>U) to an enrichment facility. The enrichment facility in turn receives requests for low enriched uranium (LEU) (4% <sup>235</sup>U) from a declared light-water reactor (ignoring the fuel fabrication facility for simplicity). The enrichment facility also receives requests for 90% enriched HEU from an undeclared actor seeking to build a nuclear weapon. Material production for each facility is calculated once each month for a total of 100 months. This framework allows us to pose the following question: If an inspector only has access to the inventory records for the LEU that arrives at the declared reactor, can diversion of material be detected?

To make the scenario more realistic, three conditions are applied to the simulation:

- The enrichment facility is operating near its maximum separative work unit (SWU) limit
- The demand for LEU material has a time-varying amplitude with a Gaussian distribution
- The enrichment facility will always prioritize fulfilling requests for HEU

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<sup>3</sup> <http://pyne.io/>

<sup>4</sup> <http://cvt.engin.umich.edu/>

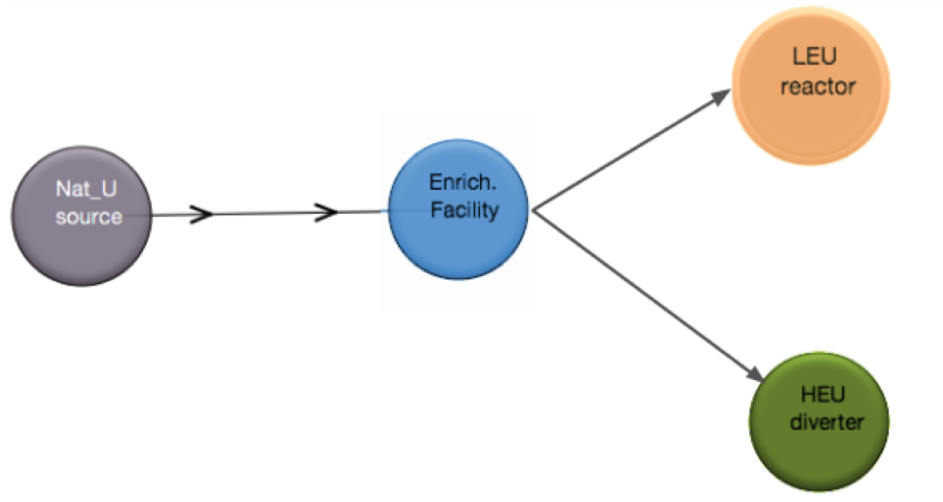


Fig. 2: Agent layout and material flow for a toy model of HEU diversion from a declared fuel cycle at the enrichment facility.

<b>General Simulation Parameters</b>	Duration (months)	100
	Natural U (% $^{235}\text{U}$ )	0.7
	LEU (% $^{235}\text{U}$ )	4.0
	HEU (% $^{235}\text{U}$ )	90.0
<b>Enrichment Facility</b>	SWU Capacity (kg-SWU/month)	180
	Tails Assay (% $^{235}\text{U}$ )	0.3
<b>LEU Demand</b>	Mean Qty (kg)	33.0
	$\sigma$ (kg)	0.5
<b>HEU Demand</b>	Qty (kg)	0.03
	Avg Rate of Occurrence	1/5

Tab. 1: Simulation parameters for HEU diversion scenario.

The SWU limit, a metric that incorporates power-consumption and maximum processing throughput, constrains the simulation so that if the enrichment facility chooses to produce HEU then its LEU output will necessarily decrease. If the LEU demand were constant then there would be a clear signature of diversion when HEU was produced. A time-variation in LEU demand is more representative of real-life, where a single enrichment facility provides fuel to many reactors, which may operate on different reloading schedules. Variations in demand can also be caused by unanticipated reactor shutdowns, delays in receiving raw material, maintenance and repairs, etc. While these events are somewhat mitigated in real operations by the use of long-term contracts and material reserves, a small variation in LEU demand is a reasonable assumption.

Several behavioral models have been explored to parameterize the behavior of the illicit actor who is requesting HEU. In the scenario presented here, the actor asks for the same quantity of material in each request, but the requests are not made at regular intervals. Rather they are modeled as occurring ‘randomly’ with a Gaussian distribution that defines their average rate of occurrence. Other models that have been examined include diversion at regular intervals, as well as independent engagement decision-making for both the illicit actor and the enrichment facility. Table 1 lists

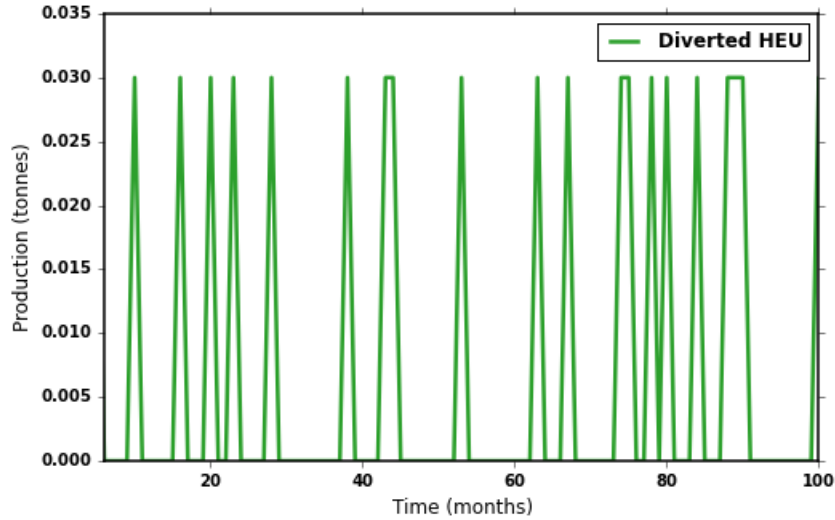


Fig. 3: An illicit actor requests HEU from the enrichment facility at random intervals with an average occurrence rate of 1 out of every 5 months.

the parameters used for the simulation, where HEU is diverted using the ‘random’ model with an average occurrence rate of once per 5 months. Figure 3 shows the HEU demand from the illicit actor as a function of time. Figure 4 illustrates the impact of this illicit material diversion on overall LEU production. The orange trace represents the amount of LEU material that would have been produced by the enrichment facility at each timestep if there had been no material diversion for HEU production. The blue trace represents the amount of LEU that was actually produced and shipped to the declared reactor during the diversion scenario.

If the inspector has access to only the blue time-series data, is it possible to identify whether or not material is being diverted from the system? A naive approach is to look at the distribution of the time-series data. Figure 5 is a histogram of the declared LEU signal showing the distribution of the quantity of LEU that was declared. The blue trace is a Gaussian fit to the declared data, while the orange trace (“expected”) is a Gaussian fit to the hypothetical variation in the LEU signal if there were no diversion. In this example, an inspector would need a sufficiently well-sampled dataset for the facility during a time when there was no diversion to characterize the expected distribution in order to draw conclusions about whether or not material diversion is occurring. An ongoing collaboration with researchers at the Michigan Institute for Data Science<sup>5</sup> seeks to apply innovative anomaly detection techniques to these simulations to investigate detection limits for scenarios with sparse data sets or low signal-to-noise ratios.

## 4 Discussion

The CYCLUS fuel cycle simulator is being used as a framework for combining techniques and knowledge from a variety of disciplines to support a cohesive approach to treaty verification. This paper presents the diversion of HEU as a simple example of measuring facility output as a treaty

<sup>5</sup> <http://midas.umich.edu/>

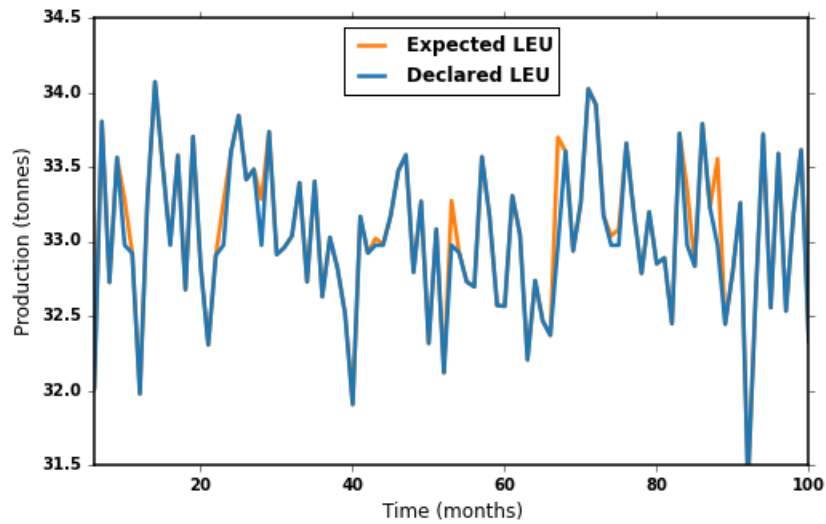


Fig. 4: Expected variation of LEU demand in the absence of diversion is shown in orange, while the LEU actually produced in the diversion scenario is shown in blue. The amplitude of the diverted material was chosen to displace the signal with one standard deviation of the expected variation.

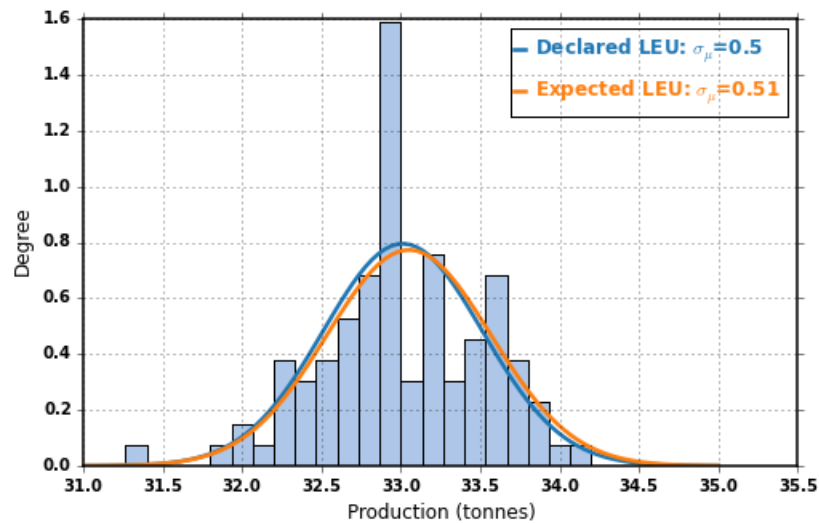


Fig. 5: Distribution of LEU quantity produced in the diversion scenario (blue). The expected variation of LEU demand in the absence of diversion is shown in orange (fitted). A shift between the fitted curves indicates that material is being diverted.



verification strategy. This HEU simulation uses a random-interval, constant-amplitude model to describe the behavior of an illicit actor seeking to divert HEU from a declared enrichment facility. It applies statistical techniques to the data that would be available to an IAEA inspector, namely the LEU production of the enrichment facility, to demonstrate that material diversion could be detected in this scenario.

This simulation is but one example of the capabilities of CYCLUS as a test bed for treaty verification strategies. CYCLUS is also being used to model the geographical dissipation of  $^{85}\text{Kr}$  emissions from a covert separations facility processing WGP in the effluent shadow of declared facilities. This feature can be used to assess the required regional distribution of various types of  $^{85}\text{Kr}$  detectors to ensure detection of clandestine reprocessing programs. Additionally, CYCLUS has the capability to produce synthetic signals of inherent physical processes such as neutron spectra of various materials. In this way, CYCLUS simulations can provide theoretical signals to researchers developing experimental detectors in order to test sensitivity and detector response.

Moving forward, CYCLUS will be used to study more complex diversion scenarios. Probabilistic models for behavior based on the actor's risk-perception will be explored. Ongoing collaborations as part of the CVT are examining the mechanisms and limits of expanding anomaly detection algorithms with other types of data, such as social media chatter. Due to the inherently interdisciplinary nature of this work, new external collaborations are sought with experts in behavioral modeling. Innovative ideas on detection modalities and diversion detection techniques are also welcomed.

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