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SAND2025-11726

SANDIA REPORT
SAND20XX-XXXX
Printed September 2025

Sandia National Laboratories

Material Control & Accounting Modeling Developments for a Generic TRISO Fuel Fabrication Facility

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ABSTRACT

The Material Protection, Accounting, and Control Technologies (MPACT) program utilizes modeling and simulation to assess Material Control and Accountability (MC&A) concerns for a variety of nuclear facilities. The Sandia National Laboratories (SNL)-developed Fissile Facility Flow Modeler (F3M) and the Material Accountancy Performance Indicator Toolkit (MAPIT) have historically provided MPACT with the capability to analyze MC&A approaches for nuclear facilities to determine that these facilities meet regulatory requirements. In FY25, improvements on the application of the F3M and MAPIT tools to simulate a generic TRi-structural ISOtropic (TRISO) fuel fabrication facility were successfully completed. The generic TRISO fuel fabrication F3M model captures the entire TRISO fuel fabrication process and is adaptable to any final TRISO fuel form, including spherical pebbles and cylindrical compacts loaded into graphite prismatic blocks. Comprehensive F3M/MAPIT functionality for the generic TRISO fuel fabrication model has been demonstrated. This modeling framework can be applied to support the U.S. Department of Energy and domestic nuclear industry stakeholders in developing MC&A approaches for advanced fuel fabrication facilities via statistical tests that demonstrate compliance to regulatory requirements.

ACKNOWLEDGEMENTS

This work was funded by the Materials Protection, Accounting, and Control Technologies (MPACT) working group as part of the Fuel Cycle Technologies Program under the U.S. Department of Energy, Office of Nuclear Energy.

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EXECUTIVE SUMMARY

This report covers the development of a new and comprehensive approach to TRi-structural ISOtropic (TRISO) fuel fabrication material control & accounting (MC&A) modeling as well as the results of key statistical tests on the flow of nuclear material throughout a generic TRISO fuel fabrication facility. This approach uses the framework of the Fissile Facility Flow Modeler (F3M), a systems-level facility simulator developed in the MATLAB Simulink framework, as well as the Material Accountancy Performance Indicator Toolkit (MAPIT), a Sandia-developed statistical test software. The modeling framework combines process variance, measurement uncertainty, and statistical tests with the standard operation cycle for a target facility. The framework can be used to determine if a facility can meet MC&A regulatory requirements.

Review of previous TRISO fuel fabrication MC&A modeling efforts have identified a need to expand the model development approach to cover the entire TRISO fuel fabrication process. Whereas previous modeling focused solely on fuel kernel processing, the approach taken in this report focuses on the entire TRISO fuel fabrication process. The fuel form chosen in this report for fuel fabrication facility MC&A statistical analysis is uranium oxycarbide (UCO) TRISO particles in an arbitrary final fuel form, which is expected to be either TRISO pebbles or TRISO cylindrical compacts loaded into prismatic blocks.

A literature review was conducted to expand on the process flows previously explored in the previous TRISO fuel fabrication facility model in the creation of a comprehensive generic TRISO fuel fabrication facility. IAEA-TECDOC-1645, "High Temperature Gas Cooled Reactor Fuels and Materials," which was developed as an educational and training document for advanced fuel developers, was used as the primary reference to construct the process flows in the new TRISO fuel fabrication F3M model. This model is shown in Figure E-1 and Figure E-2.

Each F3M block focuses on representing the tracking of uranium as it flows through the fabrication process. The generic TRISO F3M model maintains an entity list of 1,675 isotopes – the fuel fabrication processes are thus represented as additions and removals of isotopes from this entity. Only a small subset of the isotope list is tracked when modeling TRISO fuel fabrication in F3M, namely the isotopes corresponding to fresh fuel components (uranium, carbon, water etc.). These additions and removals are set based on an item mass (in kilograms). For example, an item of high assay low enriched uranium (HALEU) UO_2 feedstock would correspond to the mass of HALEU UO_2 in one drum of feedstock. The introduction of HALEU UO_2 feedstock to material balance area (MBA) 1 of the TRISO F3M model is represented by the addition of drums with a specifiable mass flowing into MBA 1 at a specifiable frequency from the HALEU UO_2 source term block. Similarly, mass flows and flow rates can be specified at each block to represent how much material flows through each process and at what frequency the material flows through each process. The TRISO F3M model incorporates chemical processes at each fabrication step through additions and removals of non-uranium elements and isotopes; waste streams are represented as fractional removals of uranium from a process block into a waste output.

The F3M/MAPIT statistical test framework is capable of supporting the development of MC&A approaches that meet regulatory requirements. This framework can calculate inventory difference (ID), standard error of the inventory difference (SEID), and SEID as a percentage of active inventory from the input, inventory, and output data from the F3M model. These statistical test results can then be compared to regulatory thresholds.

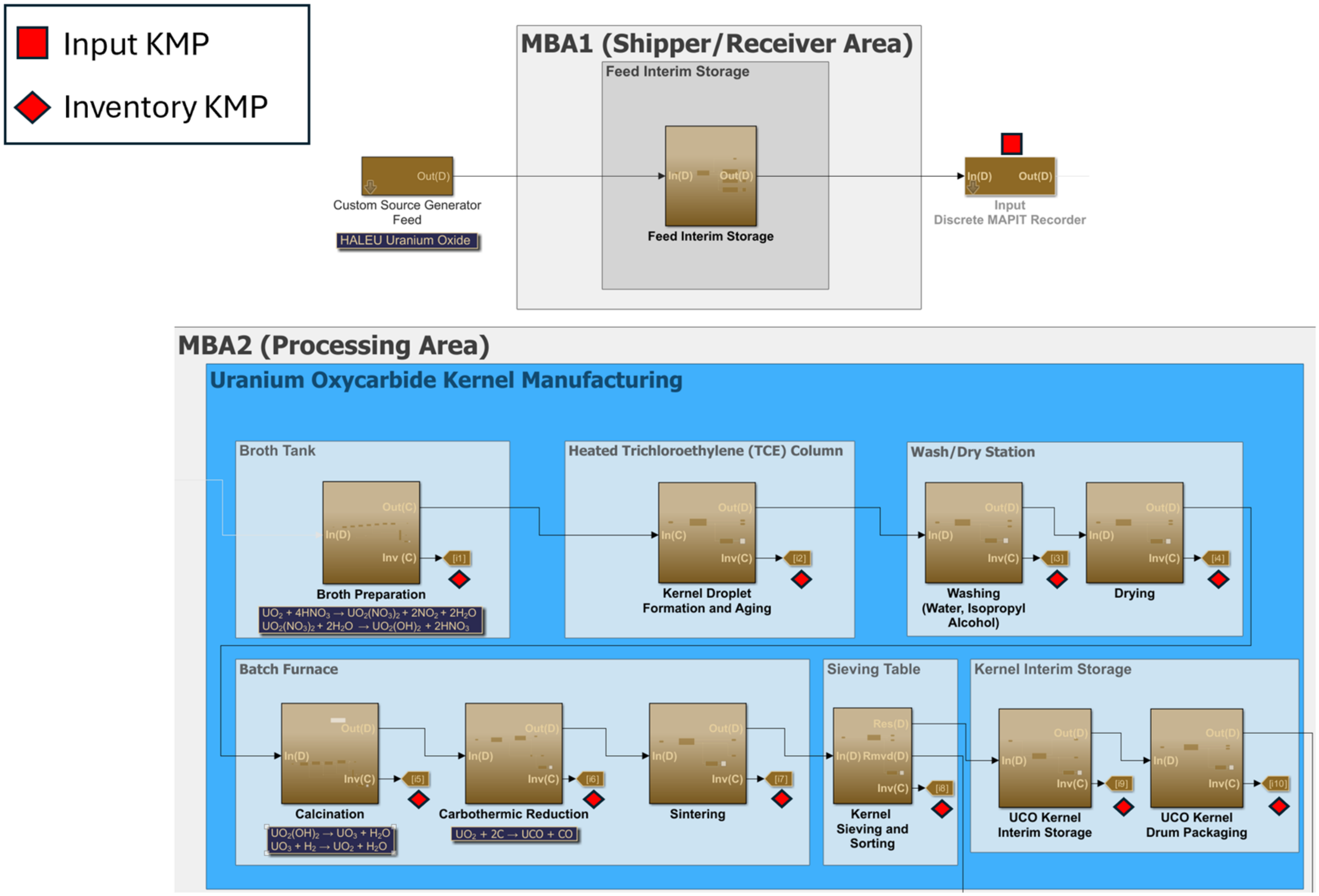

Figure E-1. The feed and kernel manufacturing sections of the generic TRISO fuel fabrication facility F3M model.

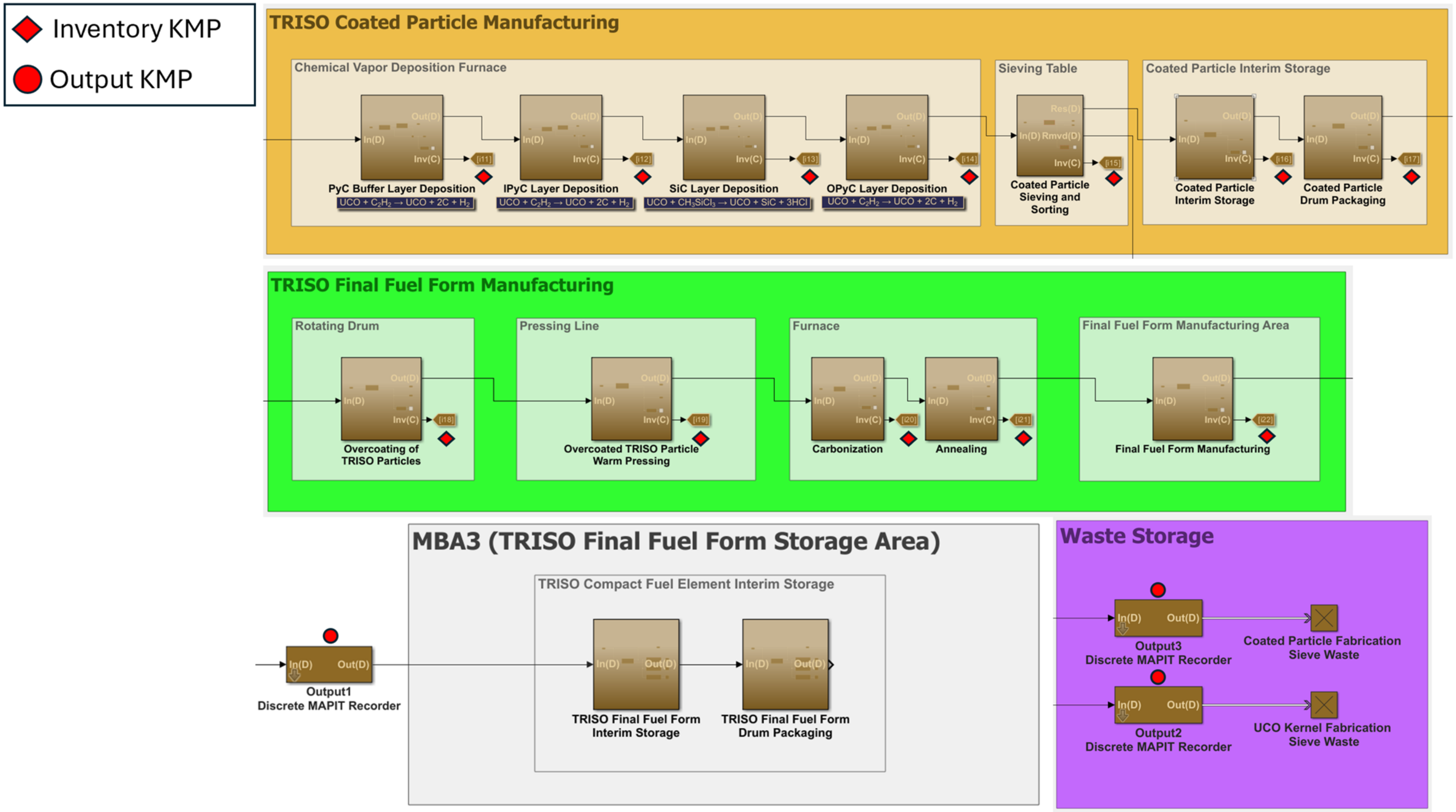

Figure E-2. The coated particle manufacturing, final fuel form manufacturing, final fuel storage, and waste storage sections of the generic TRISO fuel fabrication facility F3M model.

The regulatory requirements for a nuclear facility depend on whether the facility is under the authority of the U.S. Nuclear Regulatory Commission (NRC) or the U.S. Department of Energy (DOE). A HALEU TRISO fuel fabrication facility would likely have a special nuclear material (SNM) categorization of Category II/III under NRC regulation, or Category IV under DOE requirements, as shown in Table E-1.

Table E-1. NRC and DOE SNM categorizations expected for a TRISO fuel fabrication facility.

NRC SNM Categories (10 CFR 74)	
NRC Category II	**NRC Category III**
10,000 grams or more of ^{235}U contained in uranium enriched to 10 percent or more but less than 20 percent ^{235}U	1000 to 10,000 grams of ^{235}U contained in uranium enriched to 10 percent or more but less than 20 percent ^{235}U
DOE SNM Category (DOE Order 474.2A)	
Category IV	
Uranium containing < 20% ^{235}U, any form, any quantity	

Statistical test thresholds for meeting NRC MC&A regulatory requirements for Category II and Category III SNM facilities are given in Table E-2. Requirements for material accountancy programs are constructed to cover process areas, item accountancy, ID limits, and SEID limits. Category II requirements are summarized from 10 CFR 74.41 through 74.45 (Subpart D); Category III requirements are summarized from 10 CFR 74.31 (Subpart C).

Table E-2. Key NRC ^{235}U MC&A requirements for a fuel fabrication facility.

Requirements	Category II	Category III
Item Control Program	Detect with high probability any real loss of 300g or more of U-235	Detect with high probability any real loss of items, or uranium from items amounting to 500g or more of U-235
Control Limits for ID	Investigate and report if ID > 3 SEID or 9,000g of U-235 (Low Enriched Uranium)	90% probability of detecting a site-specific discrepancy (~1.30% of facility throughput)
Control Limits for SEID	Investigate and report if SEID > 0.125% of Active Inventory	2 (SEID) < greater of 0.25% of active inventory or 9,000g U-235
Physical Inventory Frequency	9 months	12 months

DOE-STD-1194-2019, the DOE Standard for MC&A, mentions inventory difference control limits for MBAs as follows:

> "For Category I and II, MBAs, limits-of-error of inventory differences shall not exceed a 2 percent of the active inventory during the inventory period and shall not exceed a Category II quantity of material. For Category III and IV, MBAs, limits-of-error of inventory differences shall not exceed a specified percentage of the active inventory during the inventory period to a maximum of a specified quantity; the specified percentage and maximum quantity shall be approved by DOE line management. The term "active inventory" means the sum of additions to inventory, beginning inventory, ending inventory, inventory adjustments, and removals from inventory after all "common terms" have been excluded (in this context, "common terms" are material values that appear in the active inventory calculation more than once and come from the same measurement)."

An example of F3M/MAPIT functionality is provided in Figure E-3, Figure E-4, and Figure E-5, which show ID, SEID, and SEID as a percentage of active inventory calculations, respectively, on an example generic TRISO fuel fabrication facility model. This simulation assumes 300 metric tons uranium (MTU)/year throughput processing uranium enriched to 15 wt% ^{235}U, a 4500-hour material balance period (MBP), and random and systematic uncertainties at all measurement points specified in Figure E-1 set to 1%.

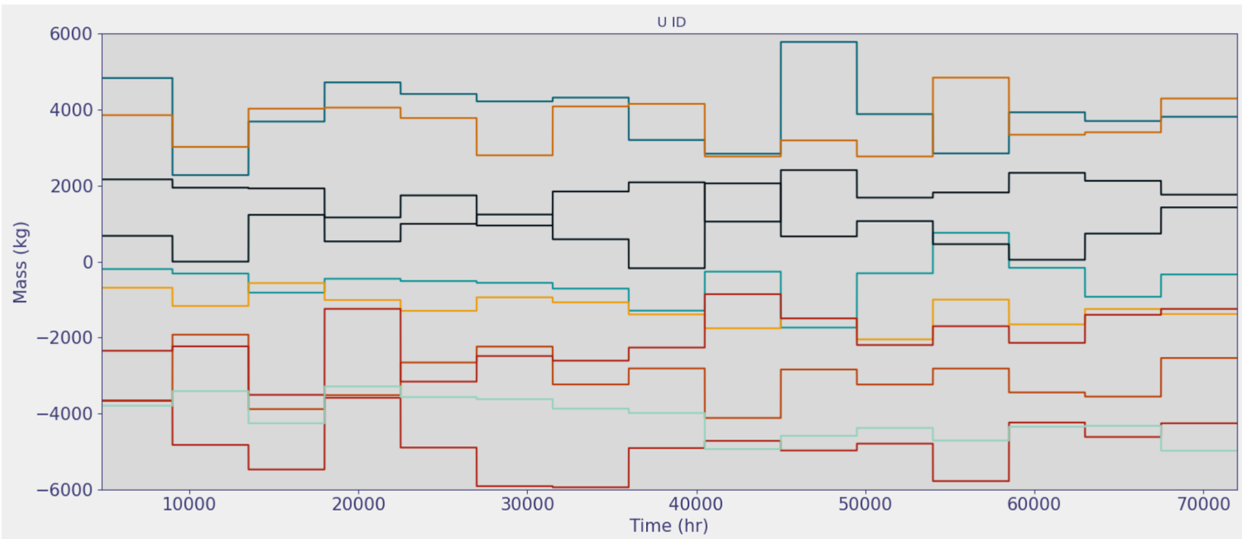

Figure E-3. MAPIT results for inventory difference of the generic TRISO fuel fabrication F3M model, with a 300 MTU/year throughput and an MBP of 4500 hours. Measurement random and systematic uncertainties are set to 1%.

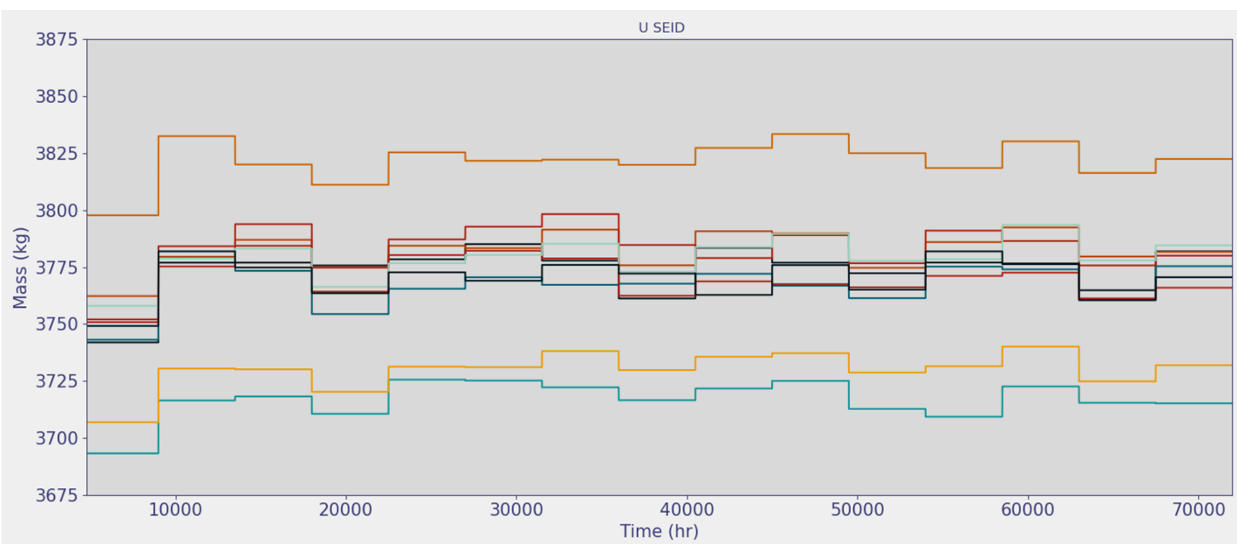

Figure E-4. MAPIT results for standard error of the inventory difference of the generic TRISO fuel fabrication F3M model, with a 300 MTU/year throughput and an MBP of 4500 hours. Measurement random and systematic uncertainties are set to 1%.

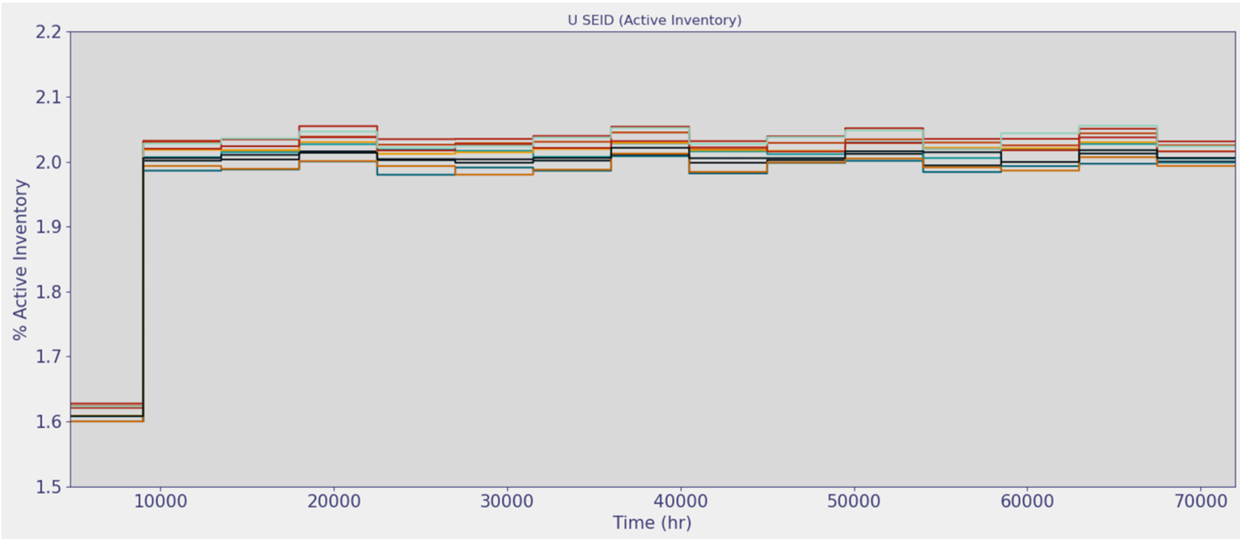

Figure E-5. MAPIT results for standard error of the inventory difference as a percentage of active inventory of the generic TRISO fuel fabrication F3M model, with a 300 MTU/year throughput and an MBP of 4500 hours. Measurement random and systematic uncertainties are set to 1%.

The results can be compared with NRC regulatory requirements listed in Table E-2 and the control limits on ID from DOE-STD-1194-2019.

- The ID fluctuations are bounded by ±6000 kg U (±900 kg of ^{235}U); the U ID is less than 3*SEID (~3*3775 kg U = 11,325 kg U), but the ^{235}U ID is greater than 9000 g (9 kg), so assuming the fuel fabrication facility is processing HALEU, this result would require an investigation per Category II requirements.
- Setting all random and systematic uncertainties to 1% results in maintaining an SEID that is ~2% of the active inventory. While this technically meets the requirements of DOE Category I and II facilities per DOE-STD-1194-2019, this does not meet the investigate and report threshold of an NRC Category II facility (SEID<0.125% of active inventory).

This methodology of simulating a TRISO fuel fabrication facility in F3M, running statistical tests in MAPIT, and comparing the statistical test results to regulatory thresholds thus demonstrates the functionality of this modeling framework.

With F3M/MAPIT functionality demonstrated, the generic F3M TRISO fuel fabrication model can now be modified to represent proposed TRISO fuel fabrication facilities, thus demonstrating its value to stakeholders such as DOE entities and industry. This value lies in both the capability to demonstrate regulatory compliance and analyze the impact of proposed measurement techniques on MC&A statistical tests to optimize facility efficiency and minimize the burden of MC&A requirements on facility operations.

ACRONYMS AND TERMS

Acronym/Term	Definition
ADU	Ammonium diuranate
CVD	Chemical vapor deposition
DOE	U.S. Department of Energy
F3M	Fissile Facility Flow Modeler
HALEU	High-assay low enriched uranium
HTGR	High temperature gas reactor
IAEA	International Atomic Energy Agency
ID	Inventory difference
IPyC	Inner pyrocarbon layer
KMP	Key measurement point
LEFFF	Low Enriched Fuel Fabrication Facility
LANL	Los Alamos National Laboratory
LEU	Low enriched uranium
LWR	Light water reactor
MAPIT	Material Accountancy Performance Indicator Toolkit
MBA	Material balance area
MBP	Material balance period
MC&A	Material control & accounting
MPACT	Materials Protection Accounting and Control Technologies
MTU	Metric tons uranium
MUF	Material unaccounted for
NRC	Nuclear Regulatory Commission
OPyC	Outer pyrocarbon layer
ORNL	Oak Ridge National Laboratory
PyC	Pyrocarbon
R&D	Research & development
SEID	Standard error of inventory difference
SiC	Silicon carbide
SNL	Sandia National Laboratories
SNM	Special nuclear material
SSBD	Safeguards and Security by Design
TCE	Trichloroethylene
TRISO	Tri-structural Isotropic
UCO	Uranium oxycarbide

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1. INTRODUCTION

The Material Protection, Accounting, and Control Technologies (MPACT) program conducts research and development (R&D) to support safeguards and security challenges for the U.S. nuclear energy program. Specifically, activities on the front- and back-end of the nuclear fuel cycle are of recent interest to the MPACT program. MPACT is focused on developing and demonstrating technologies and practices for management of nuclear material for civilian fuel cycle facilities. One goal of MPACT is the implementation of Safeguards and Security by Design (SSBD) practices, whereby safeguards and security constraints are considered early in a facility's design process, to minimize operator costs while providing the same level of performance against regulatory requirements. Opportunities for SSBD utilization are highlighted in advanced or in-development facilities, but the same techniques can be applied towards existing facilities as well.

This report covers the development of a new and comprehensive approach to TRi-structural ISOtropic (TRISO) fuel fabrication material control & accounting (MC&A) modeling as well as the results of key statistical tests on the flow of nuclear material throughout a generic TRISO fuel fabrication facility. This approach uses the framework of the Sandia National Laboratories (SNL)-developed Fissile Facility Flow Modeler (F3M), a systems-level facility simulator developed in the MATLAB Simulink framework which has been applied previously towards a variety of fuel cycle facilities, including TRISO fuel fabrication facilities [1], as well as the SNL-developed Material Accountancy Performance Indicator Toolkit (MAPIT), a Sandia-developed statistical test software. The modeling framework combines process variance, measurement uncertainty, and statistical tests with the standard operation cycle for a target facility. The framework can be used to determine if a facility can meet MC&A regulatory requirements.

1.1. Background

Advanced nuclear reactor vendors are investigating new and different approaches to energy resilience, utilizing new fuel types and higher fuel enrichment. The current nuclear fleet is primarily fueled with low enriched uranium (LEU), ^{235}U enriched to below 5%; however, new vendors are proposing higher enriched fuel in the form of high-assay low enriched uranium (HALEU), utilizing ^{235}U enriched between 5-20% [2]. The high temperature gas reactor (HTGR) utilizes TRISO particle fuel ([3], [4]) instead of traditional uranium oxide fuel assemblies.

1.2. TRISO HALEU Accountancy Challenges

New HALEU TRISO fuel fabrication facilities are in development. TRISO fuel fabrication facilities will initially have lower throughput on the order of 10-100 metric ton throughput, with proposed enrichment levels between 10-20% ^{235}U [5]. There are several domestic MC&A challenges which will need to be considered for these facilities:

- The unit processing steps for TRISO fuel fabrication are different from traditional LEU fuel fabrication.
- Differing material types associated with TRISO fuel forms require research into how well existing measurement approaches apply for accountancy and could possibly identify a need for different measurement technologies.
- The move toward HALEU fuel, which will increase the Nuclear Regulatory Commission (NRC) category of the facility to Category II.

- The material balance period (MBP) structure of the facility, which is driven by both regulatory requirements and operator choice for ease of process control.

Statistical modeling of TRISO fuel fabrication facilities simulate the statistical calculations associated with MC&A: inventory difference (ID), standard error of the inventory difference (SEID), and various statistical tests on ID calculations ([6]-[10]). The fuel fabrication facilities of light water reactors (LWRs) and HTGRs have several commonalities in terms of domestic MC&A; however, key differences may play a role in meeting regulatory requirements.

The structure of the MBAs will likely remain the same with a facility being composed of two item control areas and one processing area ([11], [12]). The item control areas are where feed material and final fuel forms entering and exiting the facility are stored, and the processing area is where the feed material is converted to the fuel form. The statistical tests for a TRISO fuel fabrication facility are the same as an LWR fuel fabrication facility; however, the material considerations and measurement techniques utilized for TRISO fuel versus LWR fuel will have key differences that will be considered in this report.

1.3. Report Focus and Structure

Review of previous TRISO fuel fabrication MC&A modeling efforts led to the identification of a need to expand the model development approach to cover the entire TRISO fuel fabrication process. Whereas previous modeling focused solely on fuel kernel processing, the approach taken in this report focuses on the entire TRISO fuel fabrication process. The fuel form chosen in this report for fuel fabrication facility safeguards statistical analysis is uranium oxycarbide (UCO) TRISO particles in an arbitrary final fuel form, which is expected to be either TRISO pebbles or TRISO cylindrical compacts loaded into prismatic blocks. UCO was chosen due to the U.S. Department of Energy (DOE) HTGR development program adoption of UCO fuel as the reference fissile particle fuel design by the early 1980s ([4], [13]), as well as UCO being the reference particle fuel design selected by X-Energy [14]. UCO fuel kernels are coated with a porous pyrocarbon (PyC) buffer layer, an inner PyC (IPyC) layer, a silicon carbide (SiC) layer, and an outer PyC (OPyC) layer.

Section 2 of this report covers the generic TRISO fuel fabrication facility model development using the F3M framework. Section 3 of this report covers the results of the statistical tests performed on the outputs of the TRISO fuel fabrication F3M model. Section 4 concludes the report with a summary of the statistical test results as well as recommendations for future TRISO fuel fabrication facility MC&A modeling efforts.

2. MODEL DEVELOPMENT

In large-throughput facilities, like a fuel fabrication plant, small measurement errors can correspond to large inventory differences. Since TRISO fuel fabrication facilities are new, there are multiple challenges including new unit operations for generation of the TRISO coated particles and final fuel forms (pebbles or compacts in prismatic blocks) as well as measurements on different fuel materials and configurations compared to existing fuel fabrication plants. Modeling and simulation provide a way to simulate and address gaps in MC&A approaches to help with current challenges facing fuel fabrication plants. Further, simulation can help determine locations where material is most likely to be lost, which can inform both inspections and ongoing research.

The new approach to TRISO fuel fabrication model development involves starting with the reference low enriched uranium (LEU) fuel fabrication facility structure shown in the International Atomic Energy Agency (IAEA) report STR 150 [11]. This reference was used to develop the material balance area structure for TRISO fuel fabrication facilities based on a reference LEU fuel fabrication facility, which can be done due to the expected similarity between fuel fabrication facility structures (two item control areas and one processing area). The reference was also used to draw from reference LEU fuel fabrication facility uranium inventory values to inform the TRISO F3M model inputs. The intent in developing the generic TRISO fuel fabrication facility is to demonstrate how differences in 1) the tracked materials in the TRISO fuel fabrication process (as compared to materials tracked during LEU fuel fabrication) and 2) the item and accounting requirements for Category II facilities would affect the MC&A statistical tests on given sensors for a generic TRISO fuel fabrication facility.

2.1. Generic TRISO Fuel Fabrication Facility Process Flow Description

A literature review was conducted to expand on the process flows explored in the previous TRISO fuel fabrication facility model [1] in the creation of a comprehensive generic TRISO fuel fabrication facility. IAEA-TECDOC-1645, "High Temperature Gas Cooled Reactor Fuels and Materials," [3] which was developed as an educational and training document for advanced fuel developers, was used as the primary reference to construct the process flows in the new TRISO fuel fabrication F3M model. This report covers the unit operations for UCO kernel manufacturing, coated particle manufacturing, and final fuel form (TRISO pebble and compact) manufacturing. The report does not cover graphite prismatic block manufacturing in great detail; however, since this safeguards modeling effort focuses on accounting for uranium in each unit operation, the operations of interest in modeling involve the fabrication of UCO kernels and TRISO coated particles – the final fuel form was not emphasized in FY25 modeling efforts and can therefore be arbitrarily chosen as either pebbles or compacts. An additional Oak Ridge National Laboratory (ORNL) reference, "Production of Low-Enriched Uranium Nitride Kernels for TRISO Particle Irradiation Testing," [15] was used to fill in information gaps on kernel droplet formation.

Figure 2-1 shows a conceptual process flow diagram of the unit operations and the material balance area structure considered for the new TRISO fuel fabrication model. In this figure, MBA 1 and MBA 3 are item control areas for fuel feedstock (HALEU UO_2) and final fuel form (UCO TRISO compact fuel element consisting of TRISO compacts loaded into graphite prismatic blocks), respectively. MBA 2 is the processing area, which for this generic facility consists of three sub-MBAs for UCO kernel manufacturing, TRISO coated particle manufacturing, and TRISO final fuel form manufacturing.

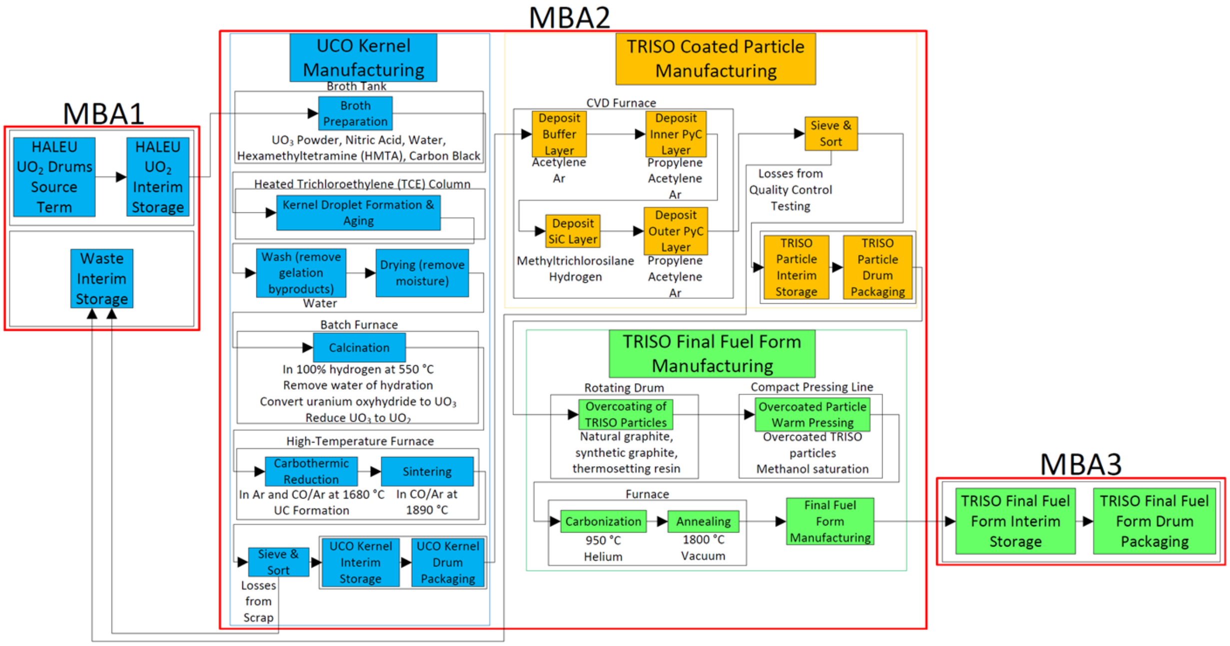

Figure 2-1. Conceptual flow diagram for TRISO fuel fabrication safeguards modeling, based on process flows described in [3]. The material balance areas are shown in red boxes.

Figure 2-2 and Figure 2-3 show the generic TRISO fuel fabrication facility developed using the F3M modeling framework in FY25 and the key measurement points (KMPs) in this model, based on the conceptual diagram in Figure 2-1. Each block in the F3M structure corresponds to a TRISO fuel fabrication process. The blocks are subdivided first into MBAs, then into various sub-MBAs corresponding to either fabrication equipment or a storage area. The intent of the model structure is to generate inputs, inventories, and outputs for the material balance calculation:

$$\mathrm{ID}_i = \sum_{l \in l_0} \int_{t=\mathrm{MBP}_{i-1}}^{\mathrm{MBP}_i} I_{t,l} - \sum_{l \in l_1} \int_{t=\mathrm{MBP}_{i-1}}^{\mathrm{MBP}_i} O_{t,l} - \sum_{l \in l_2} (C_{i,l} - C_{i-1,l})$$

Where:

- ID_i is the inventory difference of count i
- MBP_i is the material balance period of count i
- l_0, l_1, l_2 are the input, output, and inventory locations respectively
- $I_{t,l}$ is the input term at location l at time t
- $O_{t,l}$ is the output term at location l at time t
- $C_{i,l}$ is the inventory term at location l at time t
    - Note here that C is used for inventory to avoid overloaded notation between using I for both input and inventory

MAPIT can calculate ID, SEID, and SEID as a percentage of active inventory based on the input, inventory, and output data from the F3M model.

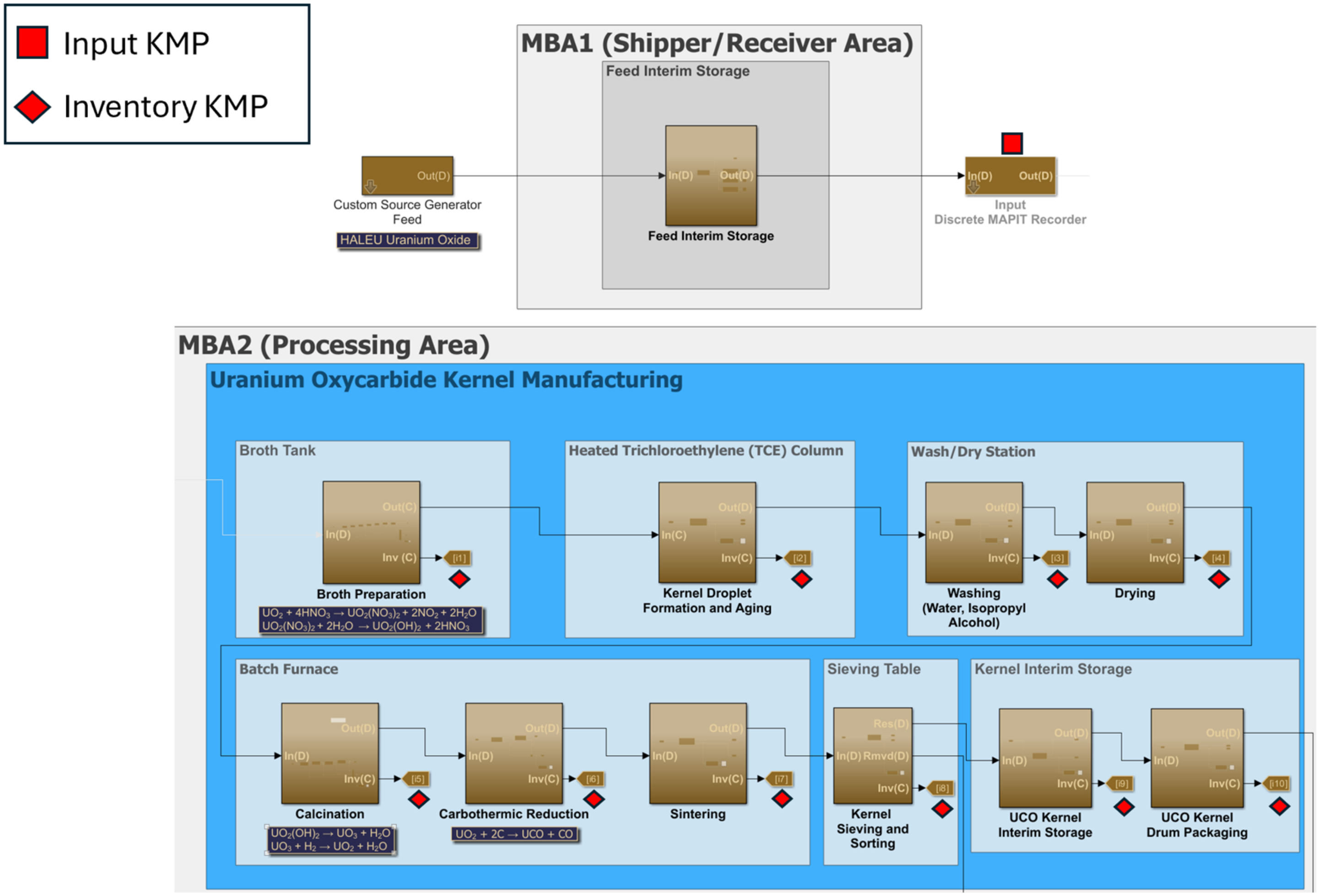

Figure 2-2. The feed and kernel manufacturing sections of the generic TRISO fuel fabrication facility F3M model developed in FY25.

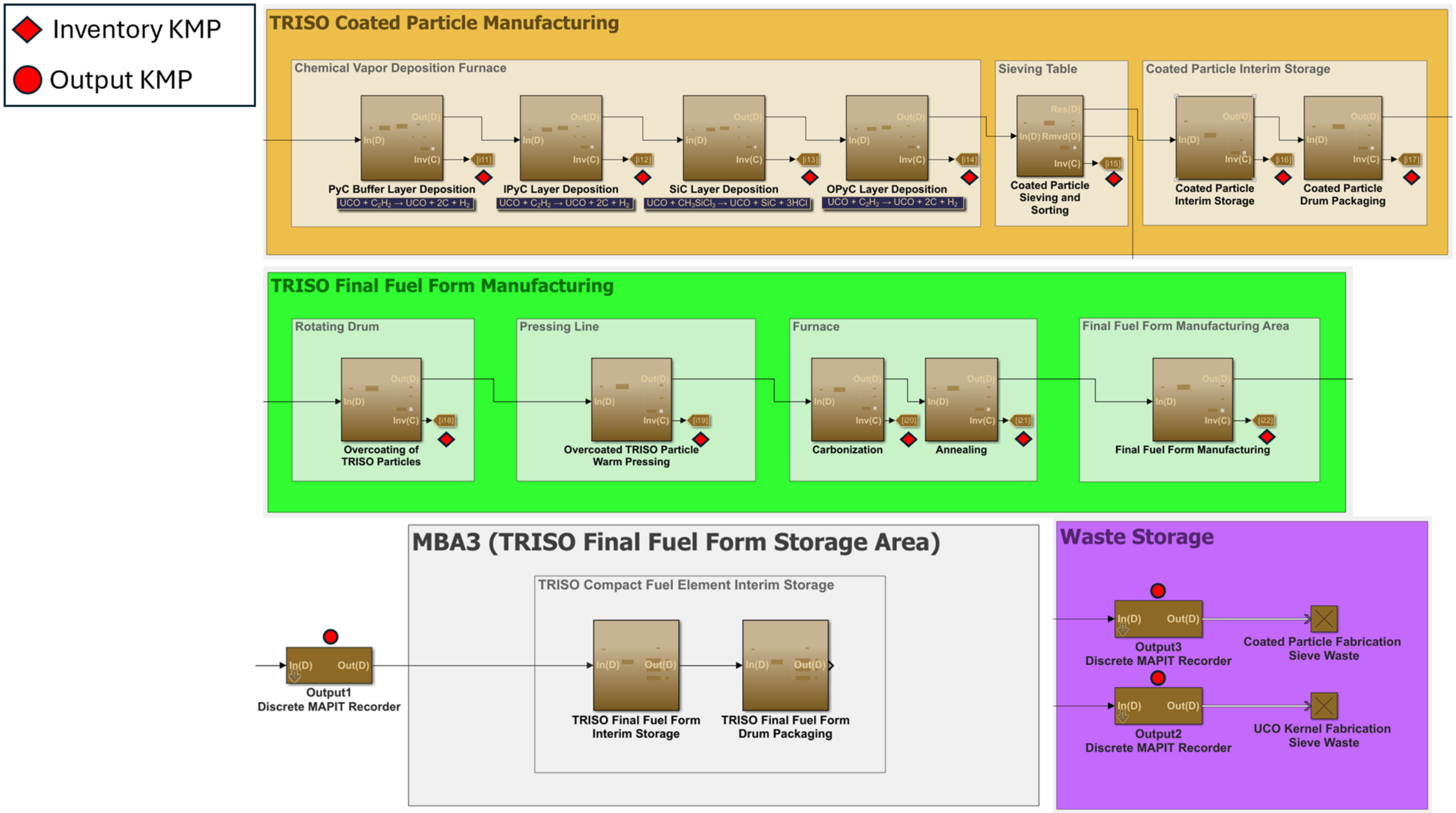

Figure 2-3. The coated particle manufacturing, final fuel form manufacturing, final fuel form storage, and waste storage sections of the generic TRISO fuel fabrication facility F3M model developed in FY25.

Continuous flows, usually expressed as mass per unit time, must be integrated over the MBP to obtain the correct terms. In contrast, discrete items can be simply summed over for each item:

$$\mathrm{ID}_i = \sum_{l \in l_0} \sum_{t=\mathrm{MBP}_{i-1}}^{\mathrm{MBP}_i} I_{t,l} - \sum_{l \in l_1} \sum_{t=\mathrm{MBP}_{i-1}}^{\mathrm{MBP}_i} O_{t,l} - \sum_{l \in l_2} (C_{i,l} - C_{i-1,l})$$

F3M allows for a combination of continuous and discrete inputs, inventories, and outputs. The only continuous inventory in the TRISO F3M model corresponds to the uranyl nitrate broth tank (the first block in MBA 2 in Figure 2-2); the rest of the inventory blocks, as well as the input and output blocks, are treated as discrete due to the tracked materials expected to be accounted for in discrete batches (drums, cans, trays etc. of material).

Each F3M block focuses on representing the tracking of uranium as it flows through the fabrication process. The generic TRISO F3M model maintains an entity list of 1,675 isotopes – the fuel fabrication processes are thus represented as additions and removals of isotopes from this entity. Only a small subset of the isotope list is tracked when modeling TRISO fuel fabrication in F3M, namely the isotopes corresponding to fresh fuel components (uranium, carbon, water etc.). These additions and removals are set based on an item mass (in kilograms). For example, an item of HALEU UO_2 feedstock would correspond to the mass of HALEU UO_2 in one drum of feedstock. The introduction of HALEU UO_2 feedstock to MBA 1 of the TRISO F3M model is represented by the addition of drums with a specifiable mass flowing into MBA 1 at a specifiable frequency from the HALEU UO_2 source term block. Similarly, mass flows and flow rates can be specified at each block to represent how much material flows through each process and at what frequency the material flows through each process. The TRISO F3M model incorporates chemical processes at each fabrication step through additions and removals of non-uranium elements and isotopes; waste streams are represented as fractional removals of uranium from a process block into a waste output.

The next few sections break down each processing step in further detail. For detailed descriptions of the variables included in the TRISO fuel fabrication F3M model, see Appendix A.

2.1.1. HALEU UO_2 feed

The flow of uranium through the generic TRISO fuel fabrication facility starts with the acceptance of HALEU UO_2 feed within MBA 1, which is representative of a feed storage area. At time zero of the modeling simulation, no uranium is present in the facility – therefore, material is first built up in MBA 1, depending on a specified storage threshold. The feed inventory within MBA 1 continues to build until reaching this threshold, after which it begins releasing items of HALEU UO_2 drums into MBA 2. The HALEU UO_2 feed section of the generic TRISO fuel fabrication F3M model is shown in Figure 2-4.

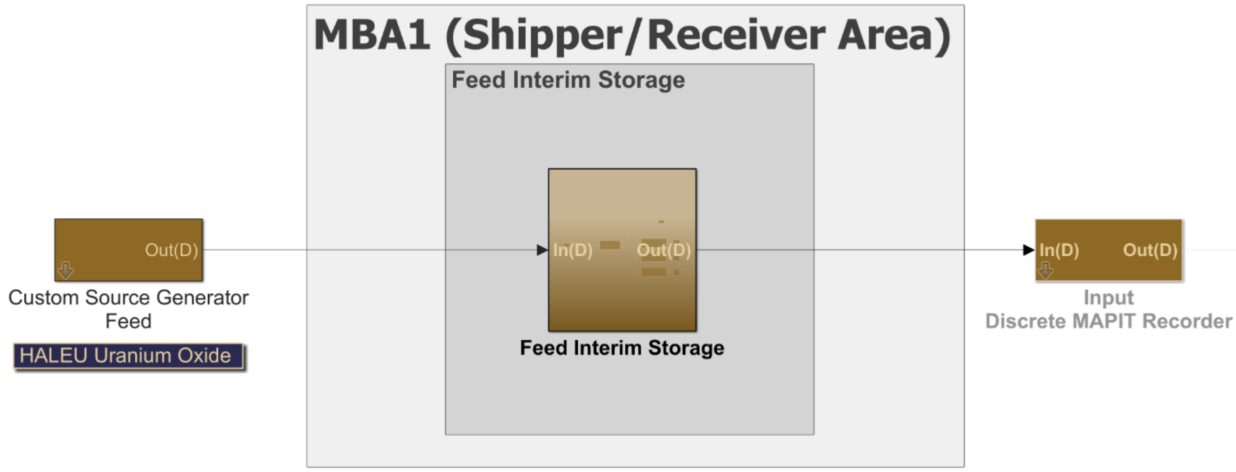

Figure 2-4. The HALEU UO_2 feed section of the TRISO fuel fabrication F3M model.

The input variables for the HALEU UO_2 feed source generator block that are in the F3M model are shown in Table A-1. The specified values for the generic model described in this report are indicated – these values are interchangeable. The resultant parameters calculated for the TRISO F3M model based on these inputs are shown in Table A-2. The feed storage area parameters are shown in Table A-3 – these parameters show that 65 drums of HALEU UO_2 feed are stored in MBA 1, and a new drum of feed is transferred for processing in MBA 2 every 24 hours.

2.1.2. UCO kernel manufacturing

The primary processing area in the generic TRISO fuel fabrication facility lies within MBA 2, per the reference fuel fabrication facility in IAEA STR 150 [11] and more recent literature on proposed TRISO fuel fabrication facility safeguards approaches [12]. The F3M model developed in FY25 focuses primarily on material balance calculations for MBA 2:

- 1 input: HALEU UO_2 feedstock drums
- 22 inventories: Inventories of uranium tracked at each processing step
- 3 outputs: Final TRISO fuel form product, waste from UCO fuel kernel production, and waste from TRISO coated particle production

Figure 2-5 shows the UCO kernel manufacturing section of the TRISO fuel fabrication F3M model. The next few sections will cover how the individual process steps are modeled in F3M, with more specific model details included in Appendix A.

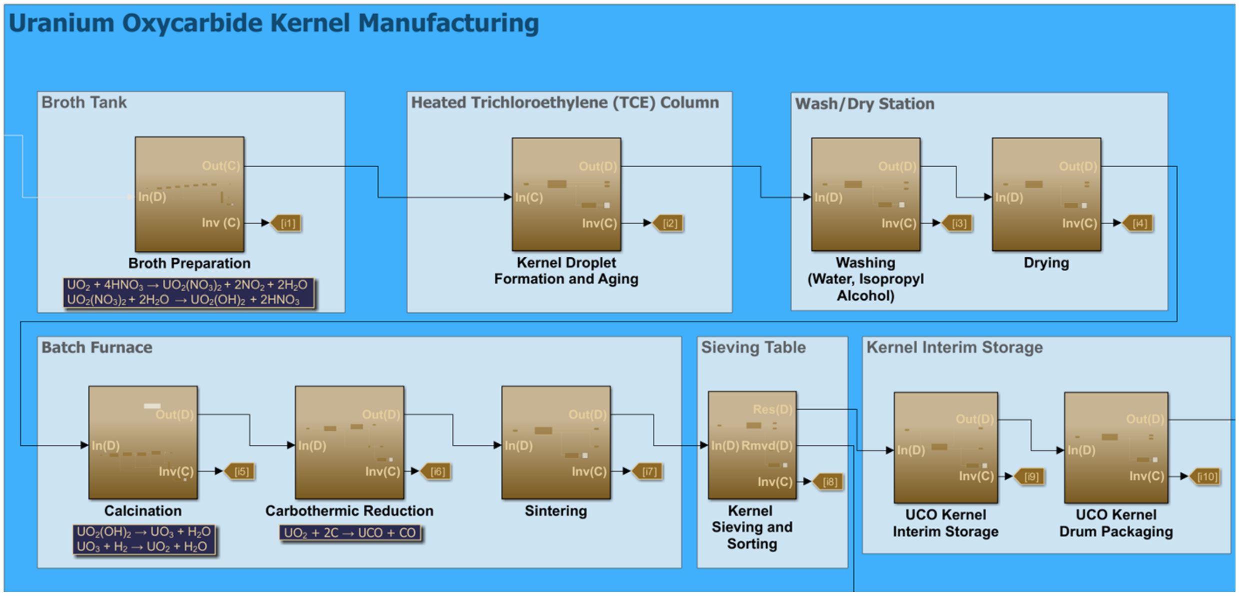

Figure 2-5. The UCO kernel manufacturing section of the TRISO fuel fabrication F3M model.

2.1.2.1. Uranyl nitrate broth preparation

The first processing step in MBA 2 is the preparation of uranyl nitrate solution. The HALEU UO_2 feed is dissolved to form the uranyl nitrate solution – this process involves an initial dissolution step, followed by neutralization (hydrolysis).

$$\text{Dissolution: } UO2 + 4HNO3 \rightarrow UO2(NO3)2 + 2NO2 + 2H2O$$

$$\text{Hydrolysis/Neutralization: } UO2(NO3)2 + 2H2O \rightarrow UO2(OH)2 + 2HNO3$$

Table A-4 shows the input variables for the uranyl nitrate broth preparation step, while Table A-5 and Table A-6 show the variables associated with the dissolution and neutralization (hydrolysis) process steps, respectively.

Seemingly redundant equations in these tables are included to separate out individual elements in each process step by mass – this information is needed to determine the mass of elements to be added or removed in each process step, which corresponds with addition and removal blocks within the F3M framework. An example of this is shown in Figure 2-6, which shows the portion of the generic TRISO fuel fabrication facility F3M model corresponding to the HALEU UO_2 dissolution step (via addition of HNO_3) in the preparation of the uranyl nitrate broth.

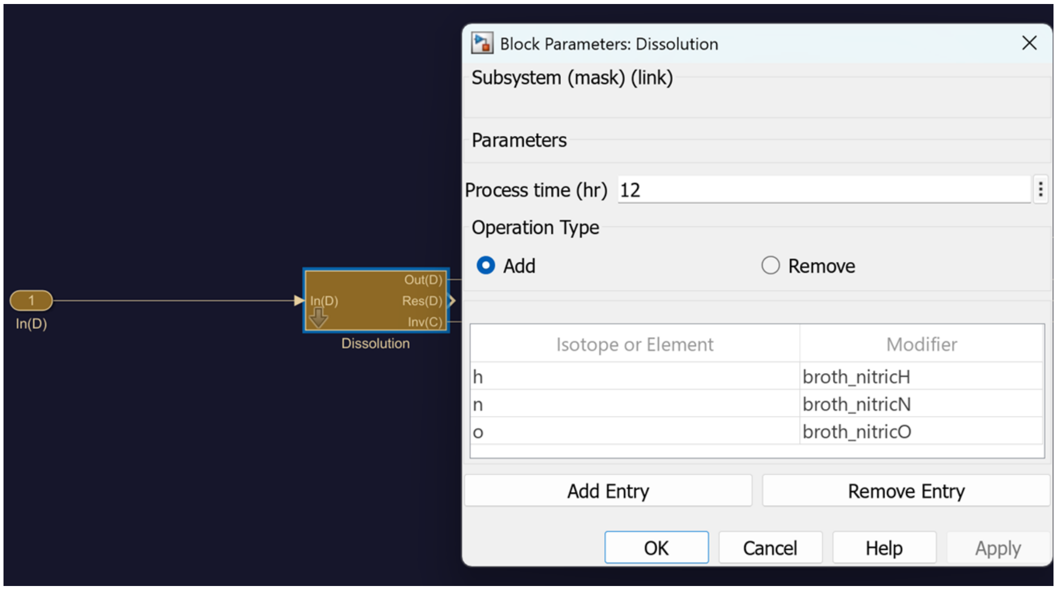

Figure 2-6. Addition block in F3M representing the HALEU UO_2 feed dissolution step in the uranyl nitrate broth preparation process.

2.1.2.2. Kernel droplet formation and aging

In this process step, the $UO_2(OH)_2$ produced from the uranyl nitrate solution is converted into droplets via a heated trichloroethylene (TCE) casting column. The TRISO F3M model neglects the chemical reactions associated with ammonium diuranate (ADU) on the droplets as well as aging; instead, the model simulates the generation of the resultant solid droplet trays from the broth flow. To maintain a constant periodicity of droplet tray outputs, the tray size (in kg) was chosen to be a multiple of the broth flow rate and arbitrarily assigned a value of ~15 kg. The kernel droplet formation and aging block parameters are shown in Table A-7.

2.1.2.3. Kernel washing and drying

The aged kernel droplets are washed first in water to remove any excess solution or contaminants, then washed in isopropyl alcohol to remove remaining moisture; the kernels are then dried through high heat and slow rotation. Since no chemical changes are expected to occur during these steps, the processes in the model are represented as simple time delays. The washing and drying block parameters are shown in Table A-8.

2.1.2.4. Kernel calcination

The dried kernel droplets are calcinated and reduced. The calcination step converts the kernels into UO_2 via the following formulas:

$$\text{Calcination: } \mathrm{UO2(OH)2} \rightarrow \mathrm{UO3} + \mathrm{H2O}$$

$$\text{Reduction: } \mathrm{UO3} + \mathrm{H2} \rightarrow \mathrm{UO2} + \mathrm{H2O}$$

The calcination step in the TRISO fuel fabrication F3M model differs from the process described in IAEA-TECDOC-1645 [3] due to the feed choice being UO_2 instead of the U_3O_8 specified in the TECDOC. The calcination block parameters are shown in Table A-9 and Table A-10.

2.1.2.5. Kernel carbothermic reduction

Following calcination, the UO_2 kernels undergo carbothermic reduction. IAEA-TECDOC-1645 describes the production of a uranium carbide product, but for the TRISO fuel fabrication F3M model, a uranium oxycarbide (UCO) product is assumed to be produced instead. The formula is taken from McMurray *et al.* [15]:

$$\text{Carbothermic Reduction: } UO2 + 2C \rightarrow UCO + CO$$

The carbothermic reduction block parameters are shown in Table A-11 and Table A-12.

2.1.2.6. Kernel sintering

Following carbothermic reduction, the kernels undergo sintering at 1890 °C to densify the kernels. Since no change in the chemical composition of the kernels occurs at this step, the TRISO fuel fabrication F3M model simulates this as an entity hold process. The only parameter under consideration here is the process time, as shown in Table A-13.

2.1.2.7. Kernel sieving and sorting

The sintered kernels undergo a sieving and sorting process using a vibrating table to select for uniform kernels. The kernels that are filtered out via sieving are taken out of processing – although these kernels could potentially be recycled to increase production efficiency, the TRISO fuel fabrication F3M model assumes that the non-uniform kernels are considered waste, and waste in this modeling framework is treated as an output from MBA 2. The parameters used to model both sieving and the resultant waste stream are shown in Table A-14.

2.1.2.8. Kernel interim storage and drum packaging

The product of the UCO kernel manufacturing sub-MBA is uniform, sintered kernels to be sent to the next processing sub-MBA, where the various coating layers (buffer PyC, IPyC, SiC, and OPyC) will be applied to the kernels. The TRISO fuel fabrication F3M model assumes that drums of kernels will be intermittently stored before moving on to the next process step; the interim storage and drum packaging parameters are shown in Table A-15.

2.1.3. Coated particle manufacturing

The next process for the fabrication of TRISO fuel is the coating of the UCO kernels. This process occurs primarily in a fluidized bed chemical vapor deposition (CVD) furnace. Following the coating process, the particles are sieved and sorted, and the uniform coated particles are transferred to TRISO final fuel form manufacturing. Figure 2-7 shows the coated particle manufacturing sub-MBA in the TRISO fuel fabrication F3M model. The next few sections will describe the coating depositions in sequence.

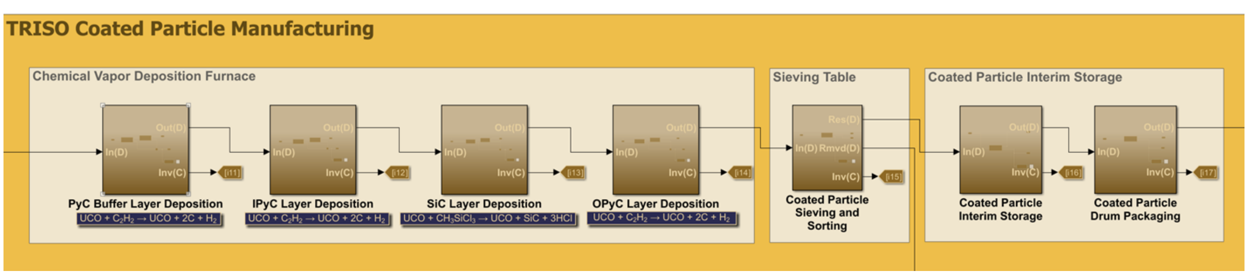

Figure 2-7. The coated particle manufacturing section of the TRISO fuel fabrication F3M model.

2.1.3.1. PyC buffer layer deposition

The first coating layer is the buffer pyrocarbon (PyC), which serves as a sacrificial layer to stop energetic fission products, protecting the IPyC layer from radiation damage, and provides void volume to accommodate fission gases and kernel swelling [3]. The buffer PyC layer is formed from the decomposition of acetylene according to the following formula [3]:

$$\text{PyC Buffer Layer Deposition: UCO} + \text{C2H2} \rightarrow \text{UCO} + 2\text{C} + \text{H2}$$

The model parameters corresponding to this first layer deposition can be found in Table A-16 and Table A-17.

2.1.3.2. IPyC layer deposition

The next coating layer is the inner pyrocarbon (IPyC) layer, which serves as a barrier against gaseous fission product diffusion and chlorine gas from the SiC deposition process [3]. The IPyC layer is deposited using a mixture of acetylene and propylene [3], but for simplicity, only acetylene is included in the TRISO fuel fabrication F3M model framework:

$$\text{IPyC Layer Deposition: UCO} + \text{C2H2} \rightarrow \text{UCO} + 2\text{C} + \text{H2}$$

The model parameters corresponding to the IPyC layer deposition are shown in Table A-18 and Table A-19.

2.1.3.3. SiC layer deposition

Following IPyC layer deposition, the silicon carbide (SiC) layer responsible for the main pressure boundary via retention of metallic fission products as well as providing durability to the TRISO particle is deposited onto the UCO kernel [3]. The SiC layer is formed by the decomposition of methyltrichlorosilane:

$$\text{SiC Layer Deposition: UCO} + \text{CH3SiCl3} \rightarrow \text{UCO} + \text{SiC} + 3\text{HCl}$$

The model parameters associated with SiC layer deposition are shown in Table A-20 and Table A-21.

2.1.3.4. OPyC layer deposition

The final coating on the TRISO particle is the outer pyrocarbon (OPyC) layer, which serves as an additional gaseous fission product barrier, reduces the tensile stress on the SiC layer, and forms a bonding surface for the overcoating material needed for manufacturing of the final TRISO fuel form [3]. The OPyC layer is formed by decomposition of acetylene, propylene, or both – for the TRISO fuel fabrication F3M model framework, much like the IPyC layer deposition, acetylene is chosen for simplicity:

$$\text{OPyC Layer Deposition: UCO} + \text{C2H2} \rightarrow \text{UCO} + 2\text{C} + \text{H2}$$

The parameters associated with this final coating are shown in Table A-22 and Table A-23.

2.1.3.5. Coated particle sieving and sorting

Following the TRISO coating process, the coated particles are once again sieved and sorted to select for uniform particles to feed into the final TRISO fuel form manufacturing process. Non-uniform coated particles are assumed to be sent to waste, which in the TRISO fuel fabrication F3M model framework is treated as an output from MBA 2. The parameters associated with coated particle sieving and sorting are shown in Table A-24.

2.1.3.6. Coated particle interim storage and drum packaging

The uniform coated particles are intermittently stored and packaged into drums for transfer to the final TRISO fuel form manufacturing sub-MBA, whether the fuel to be manufactured is spherical pebbles or cylindrical compacts. The interim storage and drum packaging parameters are shown in Table A-25.

2.1.4. Generic TRISO fuel fabrication facility model: final fuel form manufacturing

The uniform coated particles from the coated particle manufacturing sub-MBA are processed into the final TRISO fuel form, which can either be spherical pebbles or cylindrical compacts. The last portion of MBA 2 covers the manufacturing processes for the final fuel form; MBA 3 covers the storage area of the final fuel form, where the product would be expected to ship from. IAEA-TECDOC-1645 [3] contains limited details on the manufacturing of these final fuel forms – therefore, this section of the model contains the most assumptions and should be re-visited for improvements as additional information regarding these manufacturing processes is found. Figure 2-8 shows the TRISO final fuel form section of the F3M model; the next few sections go into the details that have been found for these processes as of FY25.

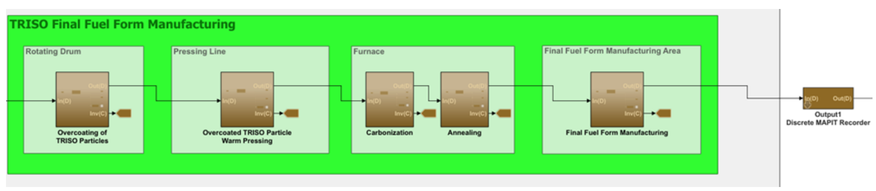

Figure 2-8. The TRISO final fuel form manufacturing section of the TRISO fuel fabrication F3M model.

2.1.4.1. TRISO particle overcoating and warm pressing

The TRISO particles are first overcoated with graphitic matrix material, which is prepared by mixing electro-graphite powder, natural graphite powder, and phenolic resin as a binder. No information on chemical formulas for these materials was provided in IAEA-TECDOC-1645 [3]. Therefore, this step is modeled as a simple time delay, as shown in Table A-26. This aspect of the model may need further development via additional information on both the chemical formulas associated with overcoating and the mass fractions of TRISO coated particles and graphitic matrix material expected during this process step.

The overcoated TRISO particles are then warm pressed into the shape of their final fuel form, whether that is spherical pebbles or cylindrical compacts. The processes and equipment used for pebbles versus compacts slightly differ; for simplification, this step is also modeled as a simple time delay, as shown in Table A-26. To expand this generic framework to model a fuel fabrication facility that specifically manufactures either pebbles or compacts, this section of the model can be updated to reflect the processes associated with manufacturing – to inform MC&A statistical tests, the mass fractions of the TRISO particles and the graphitic matrix material can be incorporated into the model in a similar fashion as was conducted for the TRISO coating layers.

2.1.4.2. Carbonization and annealing

The pressed TRISO fuel is then heated in a furnace to carbonize the phenolic resin binder, and then heated further in an annealing step to remove impurities and de-gas the fuel. These process steps are conducted for both spheres and pebbles. As with the other final TRISO fuel form manufacturing steps represented in the TRISO fuel fabrication F3M model, these process steps are modeled as simple time delays. However, since these are heat treatment steps similar to the sintering step during UCO kernel production, a time delay may actually be representative in terms of the isotopic composition of the final TRISO fuel form not changing from the previous overcoating and warm pressing steps. The carbonization and annealing process times are shown in Table A-27.

2.1.4.3. Final fuel form manufacturing

The last process step defined in MBA 2 of the TRISO fuel fabrication F3M model is a generic final fuel form manufacturing step. This could encompass the loading of TRISO compacts into graphite prismatic blocks, fuel inspections, or other processes that need to be completed prior to the final fuel product being ready to ship. Since these processes generally would not involve any associated chemical or physical changes, this process step is modeled as a simple time delay, as shown in Table A-28.

2.1.5. Waste stream outputs

The two waste streams in the generic TRISO fuel fabrication F3M model are the nonuniform particles filtered out from sieving and sorting from 1) the UCO kernel manufacturing process and 2) the TRISO coated particle manufacturing process. Although the MBA structure in the generic TRISO fuel fabrication F3M model in Figure 2-2 and Figure 2-3 considers the waste storage area as a sub-MBA within MBA 2, the model treats the waste streams as outputs from MBA 2. The waste storage sub-MBA is shown in Figure 2-9.

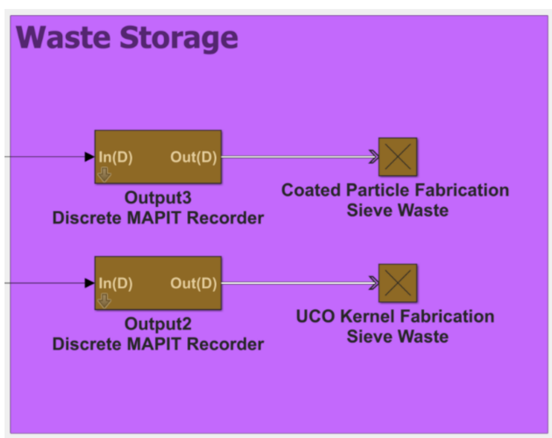

Figure 2-9. The TRISO fuel fabrication processing waste streams section of the TRISO fuel fabrication F3M model.

From Section 2.1.2.7 on kernel sieving and sorting and Section 2.1.3.5 on coated particle sieving and sorting, the assumed fraction of non-uniform kernels and coated particles (as indicated in Table A-14 and Table A-24, respectively) transferred to waste storage was both 0.002 – the quantities of these non-uniform kernels and particles are captured in the Output 2 and Output 3 Discrete MAPIT Recorders.

2.1.6. Final fuel form interim storage and drum packaging

The generic TRISO fuel fabrication F3M model assumes that the final fuel form interim storage and drum packaging area is located in MBA 3, separate from the processing MBA. As the current model structure primarily focuses on inputs, inventories, and outputs of MBA 2, MBA 3 in the model simply provides a landing area for the final TRISO fuel form output from MBA 2, which is captured by the Output 1 Discrete MAPIT Recorder as shown in Figure 2-8. The parameters for the TRISO final fuel form interim storage and drum packaging in MBA 3 are shown in Table A-29.

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3. MAPIT STATISTICAL TESTS USING GENERIC TRISO FUEL FABRICATION F3M MODEL

The generic TRISO fuel fabrication F3M model developed in FY25 includes functionality for generating input data for statistical tests in MAPIT. This section will cover how statistical tests can be used to demonstrate adherence to MC&A regulatory requirements. The section will then show how the MAPIT input data for the inputs, inventories, and outputs in MBA 2 of the TRISO fuel fabrication F3M model are generated. Finally, this section will present an example of MC&A statistical test results that can be generated using the F3M/MAPIT modeling framework.

3.1. Statistical Tests for Demonstration of Adherence to MC&A Regulatory Requirements

The F3M/MAPIT statistical test framework is capable of supporting the development of MC&A approaches that meet regulatory requirements. The regulatory requirements for a nuclear facility depend on whether the facility is under the authority of the U.S. Nuclear Regulatory Commission (NRC) or the U.S. Department of Energy (DOE).

For NRC requirements, Table 3-1 shows the NRC special nuclear material (SNM) category definitions [16], [17].

Table 3-1. NRC SNM Category Definitions.

	Category I	Category II	Category III
Strategic Significance	High	Moderate	Low
Less Than		< Category I and	< Category II and
Formula Quantity	**≥ 5000 g using**: *grams = g contained ^{235}U +2.5 (g ^{233}U + g Pu)*	**> 1,000 g combo:** *grams = g contained ^{235}U + 2 (g ^{233}U + g Pu)*	**> 15 g combo:** *grams = g contained ^{235}U + g ^{233}U + g Pu*
^{235}U (in ≥ 20% ^{235}U)	≥ 5000 g	> 1000 g	> 15 g
^{233}U or Pu	≥ 2000 g	> 500 g	> 15 g
^{235}U (in 10-20% ^{235}U)		> 10000 g	>1000 g
^{235}U (in <10% ^{235}U)			≥ 10000 g
Regulation (10 CFR 74)	Subpart E	Subpart D	Subpart C

A TRISO fuel fabrication facility would likely be Category II/III under NRC regulation, depending on facility throughput (10,000 grams or more of ^{235}U contained in uranium enriched to 10 percent or more but less than 20 percent ^{235}U for Category II; 1000 to 10,000 grams of ^{235}U contained in uranium enriched to 10 percent or more but less than 20 percent ^{235}U for Category III).

In FY24, statistical test thresholds for meeting NRC MC&A regulatory requirements for Category II and Category III SNM facilities were outlined. These requirements for facilities processing ^{235}U are given in Table 3-2. Requirements for material accountancy programs are constructed to cover process areas, item accountancy, ID limits, and SEID limits. NRC Category II requirements are summarized from 10 CFR 74.41 through 74.45 (Subpart D); Category III requirements are summarized from 10 CFR 74.31 (Subpart C) [16].

Table 3-2. Key NRC ^{235}U MC&A requirements for a fuel fabrication facility.

Requirements	Category II	Category III
Item Control Program	Detect with high probability any real loss of 300g or more of U-235	Detect with high probability any real loss of items, or uranium from items amounting to 500g or more of U-235
Control Limits for ID	Investigate and report if ID > 3 SEID or 9,000g of U-235 (LEU)	90% probability of detecting a site-specific discrepancy (~1.30% of facility throughput)
Control Limits for SEID	Investigate and report if SEID > 0.125% of Active Inventory	2 (SEID) < greater of 0.25% of active inventory or 9,000g U-235
Physical Inventory Frequency	9 months	12 months

For an NRC Category II facility, the SEID control limits and measurement uncertainty require that SEID < 0.125% of the active inventory. The ID control limits are established as a function of SEID. Thus, with an estimate of active inventory, the maximum allowable SEID and ID for a Category II facility can be calculated.

For an NRC Category III facility, the SEID control limits and measurement uncertainty are slightly less straightforward. The less restrictive of two options is chosen for two times the maximum allowable SEID: either 0.25% of active inventory or 9 kg ^{235}U (in LEU form). For a large-throughput facility, it is reasonable to assume that 0.25% active inventory >> 9 kg U-235 in LEU form. Thus, with an estimate of active inventory, the maximum allowable SEID for an NRC Category III facility can also be calculated. The control limit for ID can be estimated from the facility throughput.

For a large-throughput facility (e.g. 0.25% active inventory >> 9 kg U-235 in LEU form), both the Category II and Category III NRC requirements would dictate that the max allowable SEID is 0.125% of the active inventory. For Category II, the max allowable ID is 3*SEID or 9 kg U-235. For Category III, the maximum allowable ID can be approximated to 1.3% of annual facility throughput.

The NRC MC&A requirements apply to industry stakeholders aiming to stand up commercial-scale fuel fabrication facilities. DOE-owned facilities, such as the Low Enriched Fuel Fabrication Facility (LEFFF) at Los Alamos National Laboratory (LANL), however, are required to meet MC&A requirements under DOE Order 474.2A [18]. These requirements are based on a graded safeguards table (Table IV in [18]), which is reproduced in Table 3-3. The graded safeguards table determines both the attractiveness level (on a high to low scale from A to E) and a categorization of SNM (on a high to low scale from I to IV).

Table 3-3. DOE Order 474.2A graded safeguards table [18].

	Attractiveness Level	Pu/U-233[b] Category (kg)				Contained U-235/Separated NP-237/Separated Am-241 and Am-243 Category (kg)			
		I	II	III	IV[a]	I	II	III	IV[a]
Weapons Assembled weapons and test devices	A	All	N/A	N/A	N/A	All	N/A	N/A	N/A
Pure Products Pits, major components, button ingots, recastable metal, directly convertible materials	B	≥2	≥0.4 <2	≥0.2 <0.4	<0.2	≥5	≥1 <5	≥0.4 <1	<0.4
High-Grade Materials Carbides, oxides, nitrates, solutions (≥25 g/L) etc.; fuel elements and assemblies; alloys and mixtures; UF_4 or UF_6 (≥50% enriched)	C	≥6	≥2 <6	≥0.4 <2	<0.4	≥20	≥6 <20	≥2 <6	<2
Low-Grade Materials UF_4 or UF_6 (≥20% <50% enriched); solutions (1 to 25 g/L); process residues requiring extensive reprocessing; Pu-238 (except waste)	D	N/A	≥16	≥3 <16	<3	N/A	≥50	≥8 <50	<8
All Other Materials Highly irradiated forms, solutions (<1 g/L), compounds; uranium containing <20% U-235 or <10% U-233 (any form, any quantity)	E	N/A	N/A	N/A	Reportable Quantities	N/A	N/A	N/A	Reportable Quantities

[a]The lower limit for Category IV is equal to reportable quantities in DOE Order 474.2A.
[b]In items that contain U-233 and U-235, if the contained U-233 is 10 percent or greater of total uranium by weight, then the effective quantity of U-233 = (Contained U-233 + Contained U-235). The category is then determined by using the effective quantity of U-233 with the Pu/U-233 side of the table.

It is expected that for DOE-owned HALEU fuel fabrication facilities that plan to accept HALEU UO_2 or U_3O_8 feed, the graded safeguards table would specify that these facilities would be assigned an attractiveness level of E and therefore an SNM categorization of IV. "Reportable quantities" refer to quantities that are subject to reporting to the Nuclear Materials Management and Safeguards System (NMMSS). Guidance on reportable quantities can be found in Table I of DOE Order 474.2A [18], which is reproduced in Table 3-4.

Table 3-4. DOE Order 474.2A SNM Reportable Quantities [18].

Material Type	Reportable Quantity	Weight Field Used for Element	Weight Field Used for Isotope	Material Type Code
Enriched Uranium (U-235)	1 gram	Total U	U-235	20
Uranium-233[c]	1 gram	Total U	U-233	70
Plutonium-242[a] (Pu)	1 gram	Total Pu	Pu-242	40
Plutonium-239-241	1 gram	Total Pu	Pu-239 + Pu-241	50
Plutonium-238[b]	1/10 of a gram	Total Pu	Pu-238	83
Uranium in Cascades	1 gram	Total U	U-235	89

[a]Account as Pu-242 (Material Type (MT) 40) if the contained Pu-242 is 20 percent or greater of total plutonium by weight; otherwise, account as Pu-239-241 (MT 50)
[b]Account as Pu-238 (MT 83) if the contained Pu-238 is 10 percent or greater of total plutonium by weight; otherwise, account as Pu-239-241 (MT 50)
[c]Account as U-233 (MT 70) if the contained U-233 is 10 percent or greater of total uranium by weight; otherwise, account as U-235 (MT 10, 20, or 81).

Essentially, if the DOE-owned facility does not contain a reportable quantity of the materials listed in Table 3-4, the facility would not be subject to the requirements in DOE Order 474.2A, but it can be expected that a fuel fabrication facility would contain at least one gram of ^{235}U.

Regarding statistical controls, DOE Order 474.2A specifies the following:

> "Control limits must be established at the two-Sigma level (warning limits) and three-Sigma level (alarm limits). If two out of three consecutive data points exceed the two-Sigma level, the measurement system in question must not be used for an accountability measurement until the measurement system has been demonstrated to be within statistical control. If a single data point exceeds the three-Sigma level, the measurement system in question must not be used for an accountability measurement until the measurement system has been demonstrated to be within statistical control."

DOE Order 474.2A also specifies required physical inventory periods for the various SNM categories, as shown in Table 3-5.

Table 3-5. DOE Order 474.2A physical inventory periods [18].

Category	Processing MBA	Storage MBA
I	2 months	6 months
II	2 months	6 months
III	6 months	2 years
IV	2 years	2 years

DOE-STD-1194-2019 [19] mentions inventory difference control limits for MBAs as follows:

> "For Category I and II, MBAs, limits-of-error of inventory differences shall not exceed a 2 percent of the active inventory during the inventory period and shall not exceed a Category II quantity of material. For Category III and IV, MBAs, limits-of-error of inventory differences shall not exceed a specified percentage of the active inventory during the inventory period to a maximum of a specified quantity; the specified percentage and maximum quantity shall be approved by DOE line management. The term "active inventory" means the sum of additions to inventory, beginning inventory, ending inventory, inventory adjustments, and removals from

inventory after all "common terms" have been excluded (in this context, "common terms" are material values that appear in the active inventory calculation more than once and come from the same measurement)."

From this description, it is unclear what the specified percentage of the active inventory and maximum quantity to be approved by DOE line management could be. However, the SNL-developed statistical modeling tools can be used to inform development of an MC&A system to ensure appropriate control of nuclear material.

MAPIT has the capability to analyze ID, SEID, and SEID as a percentage of active inventory for simulated facilities; the last parameter can be compared to the inventory difference control limits specified in DOE-STD-1194-2019 [19]. This process can assist with the demonstration of adequate statistical controls for a DOE-owned fuel HALEU fabrication facility. The generic TRISO fuel fabrication F3M model can specify a simulation period that can account for multiple MBAs of any length. Therefore, the F3M/MAPIT modeling framework has the capability to demonstrate how both NRC-regulated and DOE-owned fuel fabrication facilities can meet the statistical control limit thresholds under their respective MC&A regulatory requirements.

3.2. Generation of MAPIT Inputs from F3M

The statistical tests calculated in MAPIT are based on simulations of the TRISO fuel fabrication facility modeled in F3M. The simulation run time represents how long the fabrication facility operates for, with zero elapsed time corresponding to the initial start-up of the facility. The model is structured to generate inputs, inventories, and outputs in the processing area of the fuel fabrication facility, which is chosen to be MBA 2 in the F3M model. The inputs, inventories, and outputs in the model shown in Figure 2-2 and Figure 2-3 are listed in Table 3-6.

Table 3-6. Inputs, inventories, and outputs generated from the generic TRISO fuel fabrication F3M model.

Data Type	F3M Tag	Variables
Input	Input	Feed
Inventory	out.loc1_inventory1	Uranyl nitrate broth
	out.loc1_inventory2	Kernel droplet formation and aging
	out.loc1_inventory3	Kernel washing
	out.loc1_inventory4	Kernel drying
	out.loc1_inventory5	Kernel calcination
	out.loc1_inventory6	Kernel carbothermic reduction
	out.loc1_inventory7	Kernel sintering
	out.loc1_inventory8	Kernel sieving and sorting
	out.loc1_inventory9	Kernel interim storage
	out.loc1_inventory10	Kernel drum packaging
	out.loc1_inventory11	PyC buffer layer deposition
	out.loc1_inventory12	IPyC buffer layer deposition
	out.loc1_inventory13	SiC layer deposition
	out.loc1_inventory14	OPyC layer deposition

Data Type	F3M Tag	Variables
	out.loc1_inventory15	Coated particle sieving and sorting
	out.loc1_inventory16	Coated particle interim storage
	out.loc1_inventory17	Coated particle drum packaging
	out.loc1_inventory18	Overcoating of TRISO particles
	out.loc1_inventory19	Overcoated TRISO particle warm pressing
	out.loc1_inventory20	TRISO fuel carbonization
Inventory	out.loc1_inventory21	TRISO fuel annealing
	out.loc1_inventory22	Final fuel form manufacturing
Output	Output1	Final fuel form product to interim storage
	Output2	Kernel waste
	Output3	Coated particle waste

3.3. MAPIT Statistical Test Setup

3.3.1. Reading F3M data into MAPIT

The Discrete MAPIT Recorder blocks for the inputs and outputs, as well as the inventory tag blocks, represent instrumentation at each KMP in Figure 2-2 and Figure 2-3. These blocks generate data which can then be saved as MAPIT input files via a MAPIT extractor script, which can be distributed to users of this modeling framework by contacting the report authors. The `.mat` files (`in.mat, invn.mat, and outn.mat`) need to be saved in individual folders to be properly read into MAPIT, as shown in Figure 3-1.

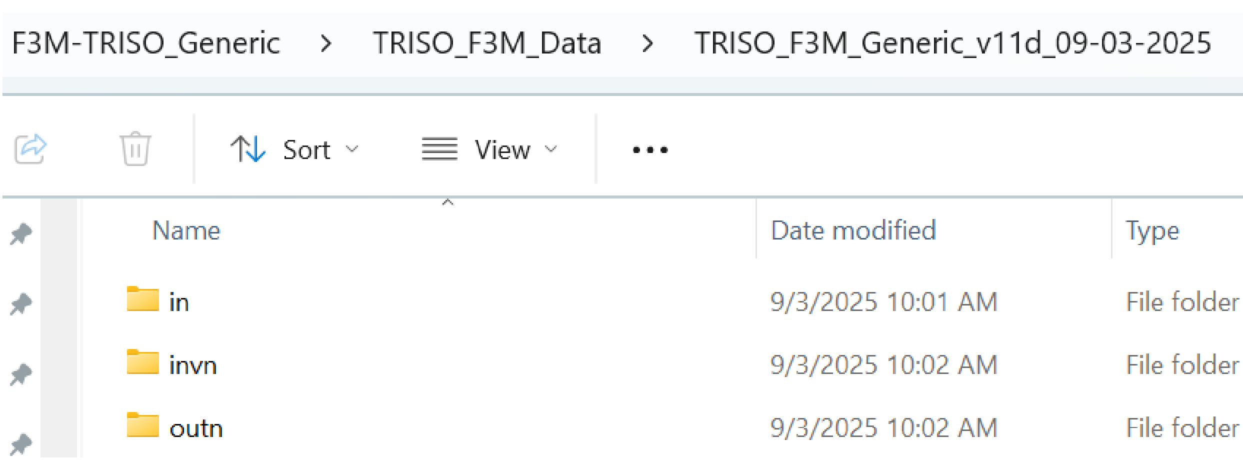

Figure 3-1. Generation of MAPIT inputs using the MAPIT extractor script. Each .mat file needs to be saved in its own individual folder to be properly read into MAPIT.

Once the `.mat` files from the F3M model are generated, these files can be read into MAPIT by selecting "Load External Data" at the top left of the MAPIT user interface, and then units and labels can be entered as shown in Figure 3-2.

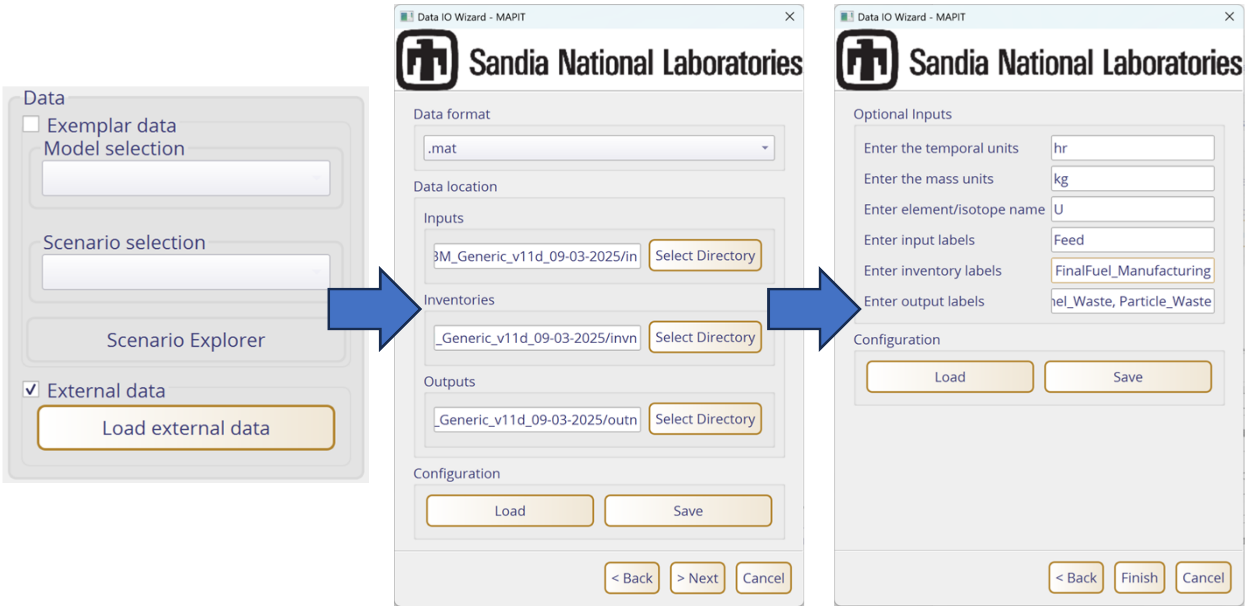

Figure 3-2. Loading external data from the TRISO fuel fabrication F3M model into MAPIT.

3.3.2. Material balance period and temporal offset selection

To optimize the choice of material balance period, the F3M data can be analyzed to determine an MBP periodicity which would correspond to minimal impacts to facility operations. For this modeling framework, this manifests in the selection of an MBP that corresponds to periods in the fabrication process where all inventories at the time in which a material balance would occur are at local minimums, corresponding to an MBP where the least number of KMPs contain nuclear material. The process flows in the generic model demonstration were assigned arbitrary processing times, as shown in Appendix A. An MBP checker script was created to count all non-zero inventories as a function of time and can be provided to users of this F3M/MAPIT framework by contacting the report authors. The choice of MBP would thus correspond to a periodicity in which the non-zero inventory count is constant at every MBP, as shown in Figure 3-3.

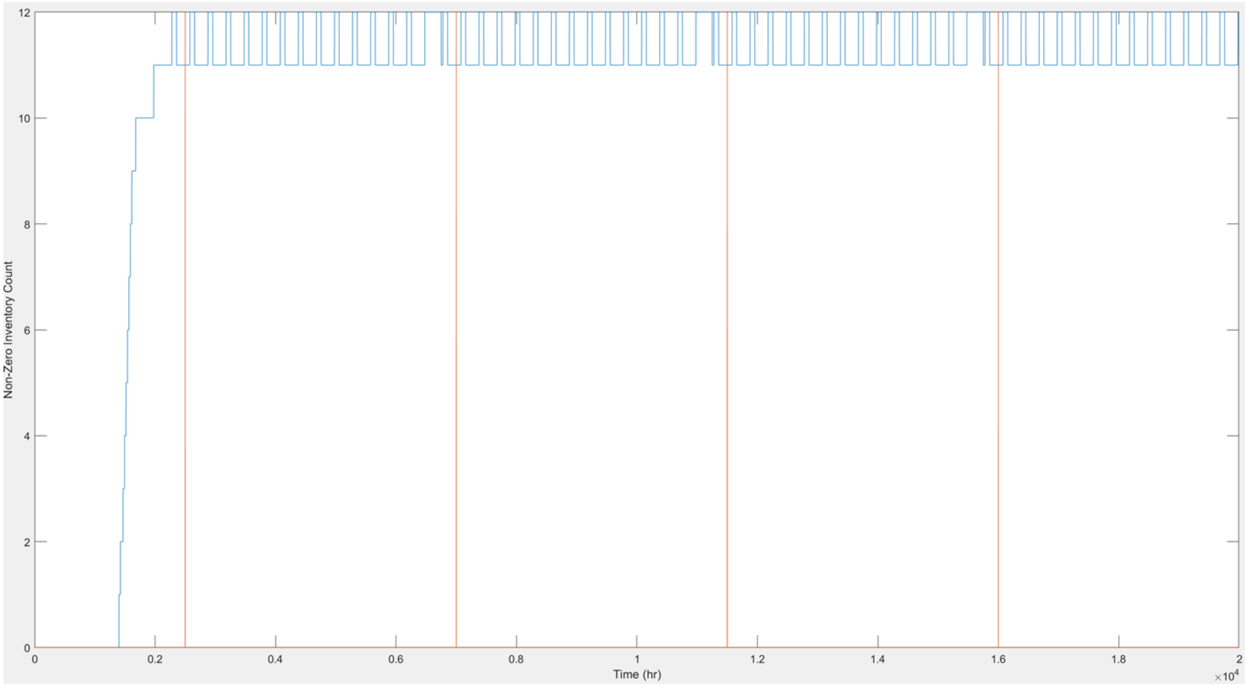

Figure 3-3. Application of the MBP checker script to determine an appropriate material balance period for a TRISO fuel fabrication facility. Blue lines represent non-zero inventory count as a function of time; orange lines represent the MBP choice. The MBP is set to 4500 hours, while the temporal offset is set to 2500 hours.

MC&A statistical test analyses of interest can be selected in MAPIT, as shown in Figure 3-4. Note that material unaccounted for (MUF) and sigma MUF are interchangeable with ID and SEID, respectively. For literature pertaining to how these statistical tests are calculated, the publicly available MAPIT site on Github [20] provides the theoretical background needed to understand how the statistical tests are calculated.

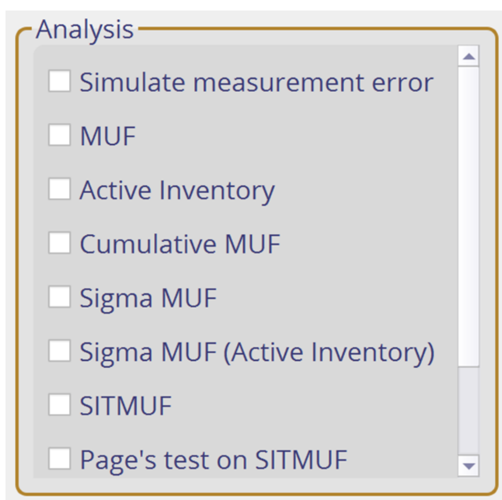

Figure 3-4. Selection of statistical tests to be analyzed in MAPIT.

In MAPIT, the MBP for MC&A statistical test analyses, as well as the number of iterations of each calculation specified per Figure 3-4, the element to be analyzed (which for MC&A statistical tests is typically uranium), and a temporal offset can be selected in MAPIT, as shown in Figure 3-5. At zero elapsed time, uranium is first introduced into the facility via the HALEU uranium oxide custom source generator in Figure 2-4. Based on the process times specified at each step of the generic TRISO fuel fabrication F3M model, a sufficiently long simulation run time is needed to allow material to flow through the entire facility; otherwise, the MAPIT extractor script will not function properly. The temporal offset allows for a simplified method of simulating material balance periods during normal operating conditions beyond the initial transient of material introduction by offsetting the entire period in which material is first introduced.

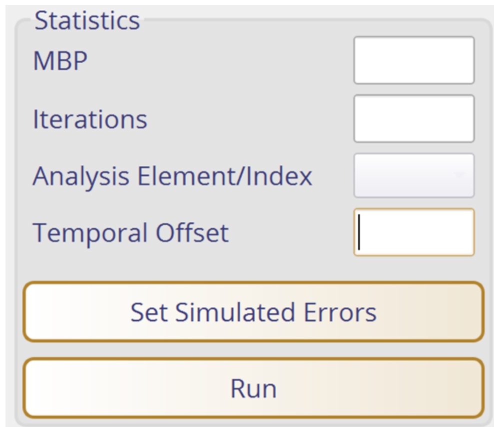

Figure 3-5. Selection of the material balance period, number of statistical test iterations, the element to be analyzed (typically uranium or U for MC&A analyses) and addition of a temporal offset to the F3M simulation period in MAPIT to represent normal operating conditions following the initial introduction of nuclear material.

3.4. Demonstration of MAPIT Statistical Tests from Generic TRISO Fuel Fabrication F3M Model

This section will present results from utilizing the generic TRISO fuel fabrication F3M/MAPIT modeling framework to generate statistical tests analyses that support the demonstration of a fuel fabrication facility's compliance with MC&A regulatory requirements. The demonstration utilizes all inputs, inventories, and outputs listed in Table 3-6. The key parameters included in this demonstration are shown in Table 3-7.

Table 3-7. Key parameters for generic TRISO fuel fabrication model demonstration using all 22 inventories.

Parameter	Value	Units
Facility throughput	300	Metric tons uranium (MTU)/year
^{235}U enrichment	15	percent

MAPIT outputs for ID, SEID, and SEID as a percentage of active inventory for the generic TRISO F3M model with a material balance period of 4500 hours (~6 months) are shown in Figure 3-6, Figure 3-7, and Figure 3-8, respectively.

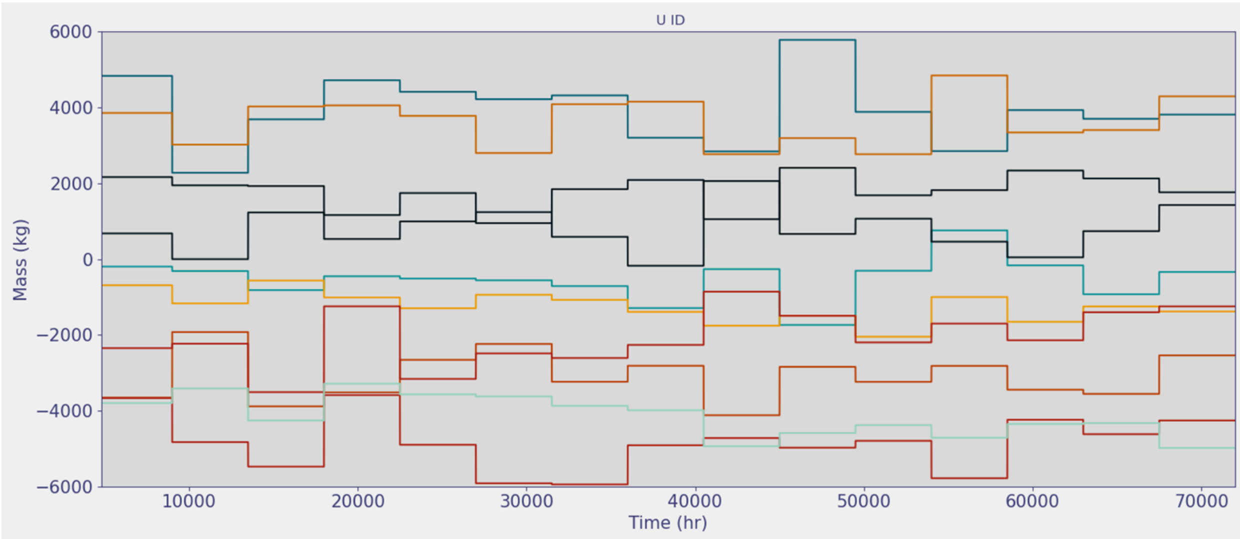

Figure 3-6. MAPIT results for inventory difference of the generic TRISO fuel fabrication F3M model, with an MBP of 4500 hours and random and systematic uncertainties at every KMP set to 1%.

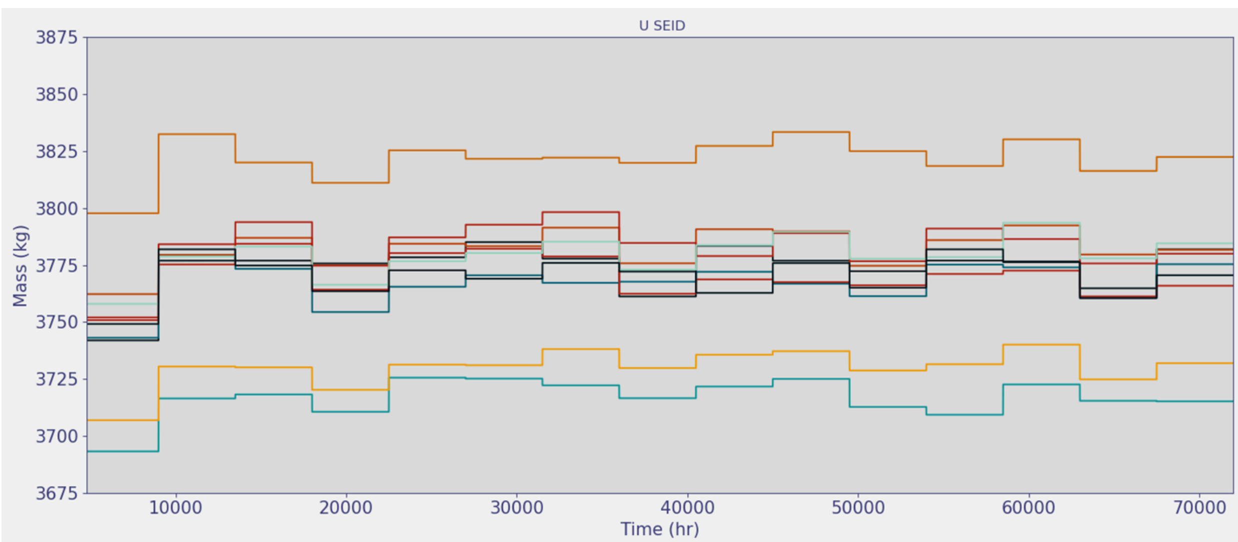

Figure 3-7. MAPIT results for standard error of the inventory difference for the generic TRISO fuel fabrication F3M model, with an MBP of 4500 hours and random and systematic uncertainties at every KMP set to 1%.

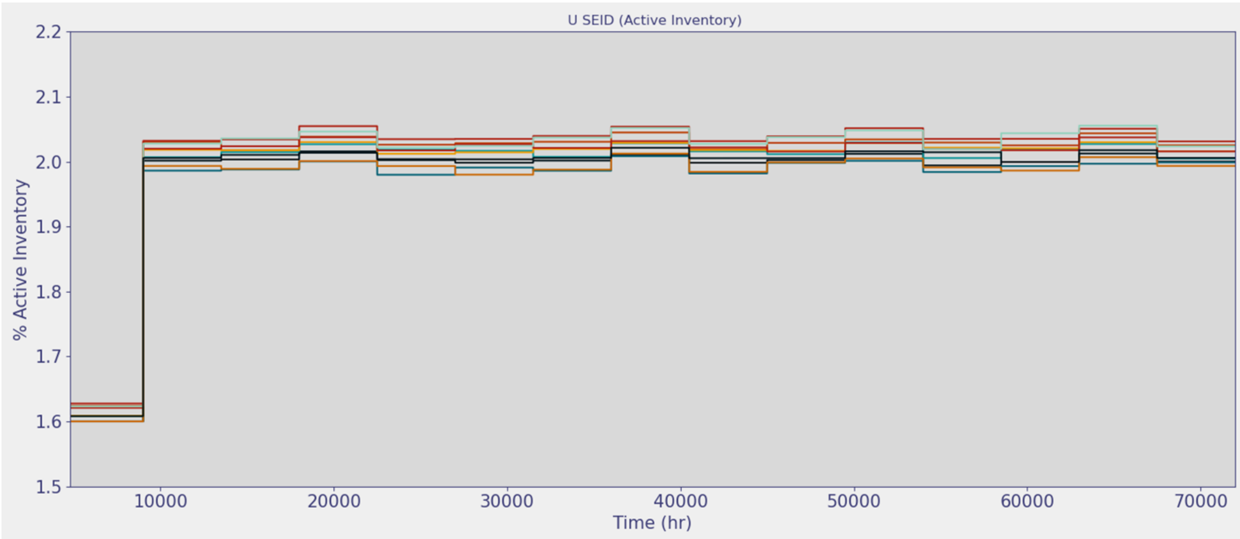

Figure 3-8. MAPIT results for standard error of the inventory difference as a percentage of active inventory for the generic TRISO fuel fabrication F3M model, with an MBP of 4500 hours and random and systematic uncertainties at every KMP set to 1%.

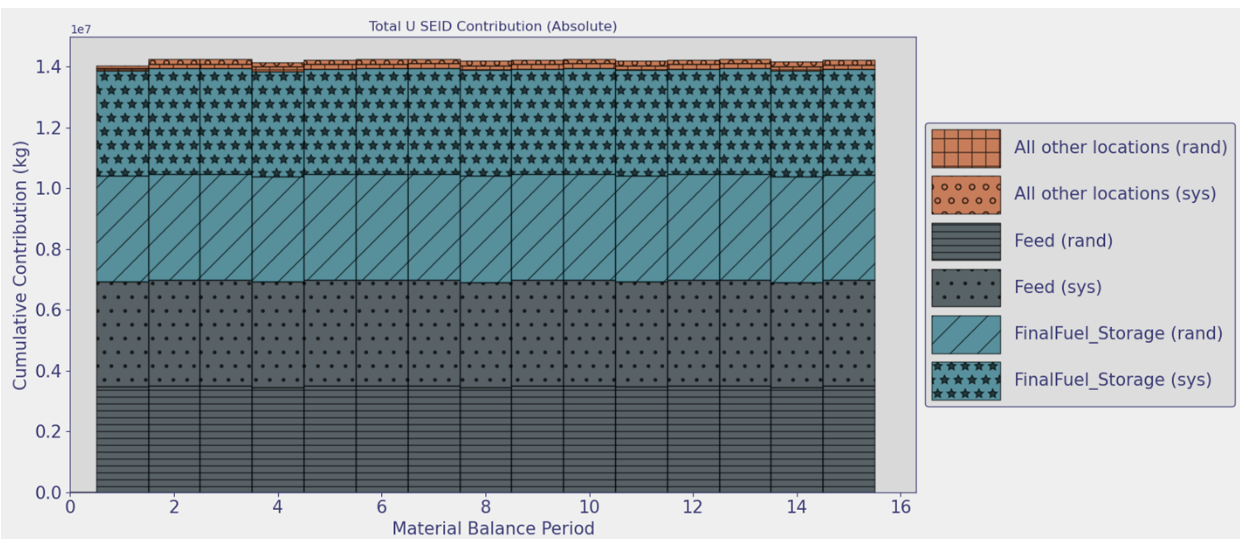

Figure 3-9. MAPIT results for measurement point contributions to standard error of the inventory difference for the generic TRISO fuel fabrication F3M model, with an MBP of 4500 hours and random and systematic uncertainties at every KMP set to 1%.

Comparison of these results with NRC Category II requirements listed in Table 3-2 and the control limits on ID from DOE-STD-1194-2019 [19] give the following conclusions:

- The ID fluctuations are bounded by ±6000 kg U (±900 kg of ^{235}U); the U ID is less than 3*SEID (~3*3775 kg U = 11,325 kg U), but the ^{235}U ID is greater than 9000 g (9 kg), so this result would require an investigation.
- Setting all random and systematic uncertainties to 1% results in maintaining an SEID that is ~2% of the active inventory. While this technically meets the requirements of DOE Category I and II facilities per DOE-STD-1194-2019 [19], this does not meet the investigate and report threshold of an NRC Category II facility (SEID<0.125% of active inventory).

An analysis of how the choice of material balance period affects the statistical tests is demonstrated in the following section. Changing the MBP to 17,400 hours (~2 years), corresponding to SNM Category IV physical inventory period requirements listed in Table 3-5, results in the following changes to ID, SEID, SEID as a percentage of active inventory, and the contributions to SEID, as shown in Figure 3-10, Figure 3-11, Figure 3-12, and Figure 3-13, respectively.

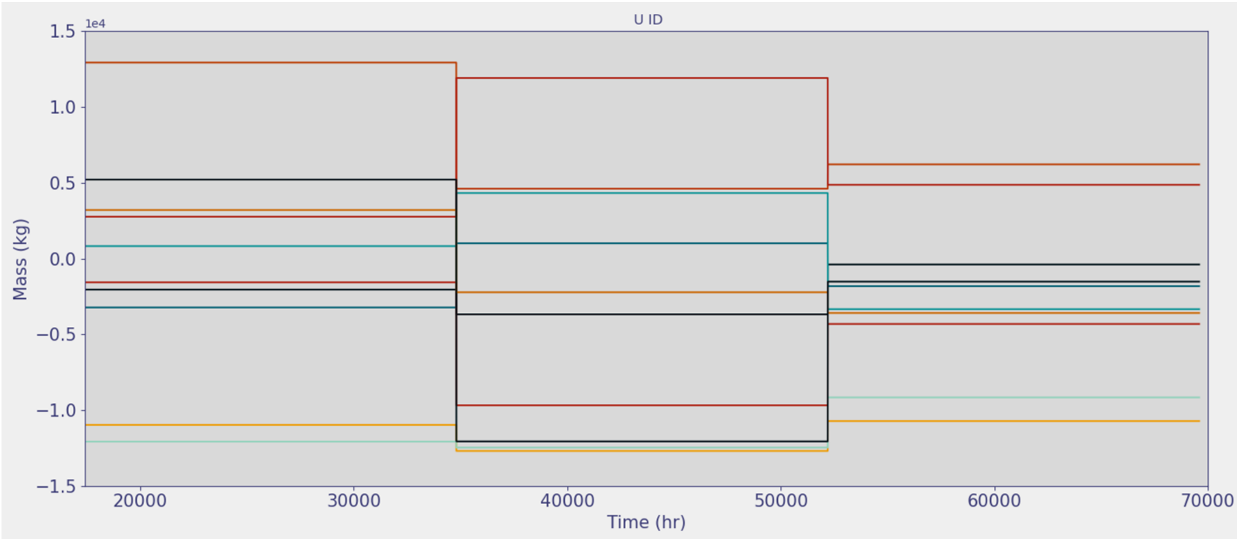

Figure 3-10. MAPIT results for inventory difference of the generic TRISO fuel fabrication F3M model, with an MBP of 17,400 hours and random and systematic uncertainties at every KMP set to 1%.

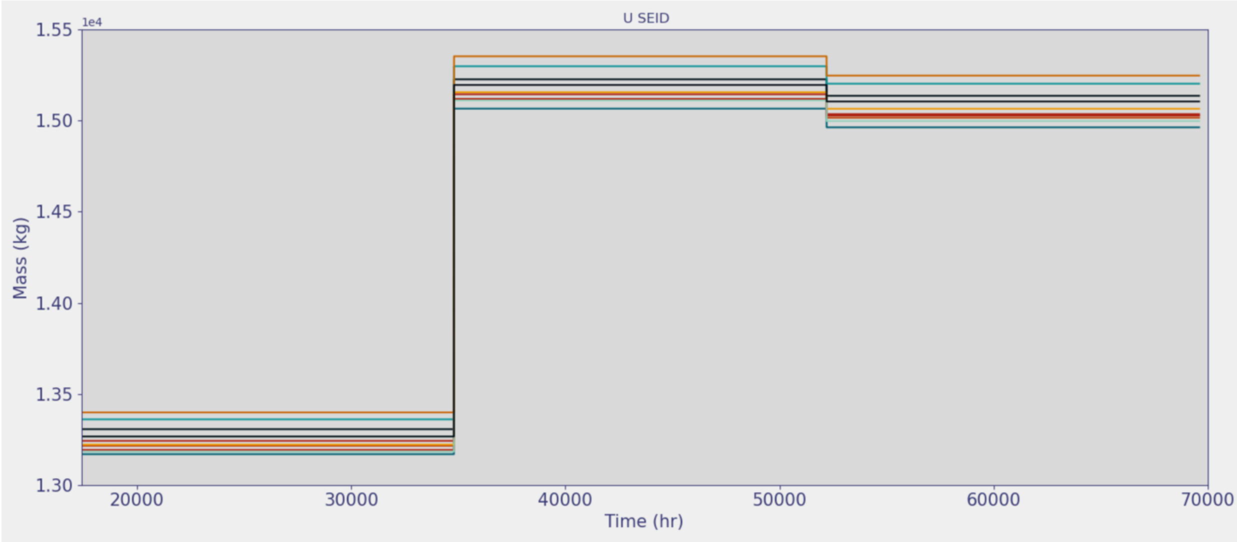

Figure 3-11. MAPIT results for standard error of the inventory difference for the generic TRISO fuel fabrication F3M model, with an MBP of 17,400 hours and random and systematic uncertainties at every KMP set to 1%.

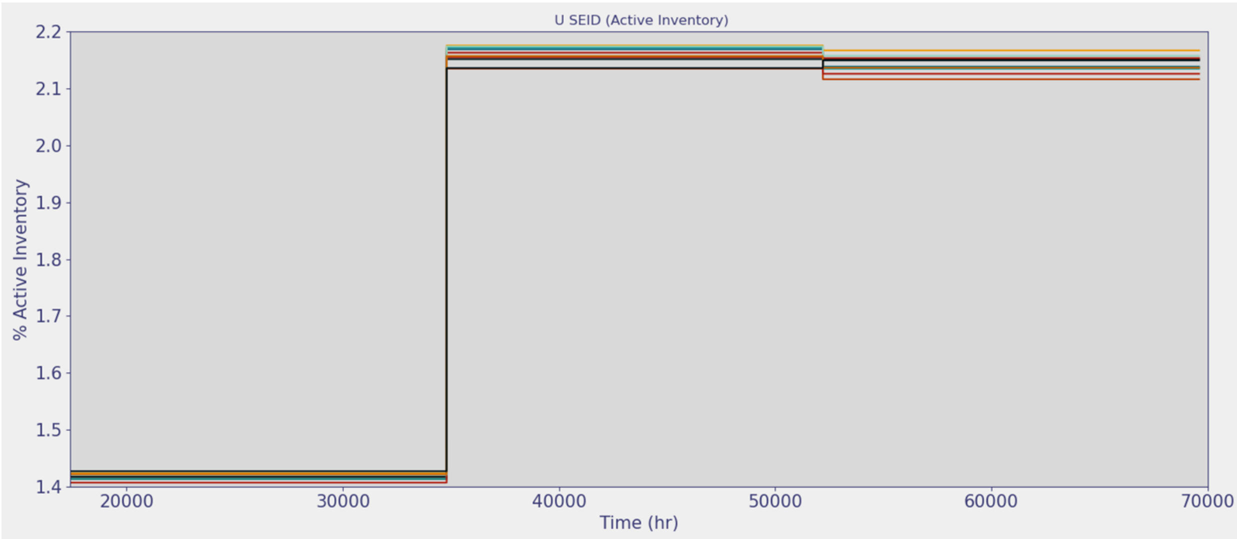

Figure 3-12. MAPIT results for standard error of the inventory difference as a percentage of active inventory for the generic TRISO fuel fabrication F3M model, with an MBP of 17,400 hours and random and systematic uncertainties at every KMP set to 1%.

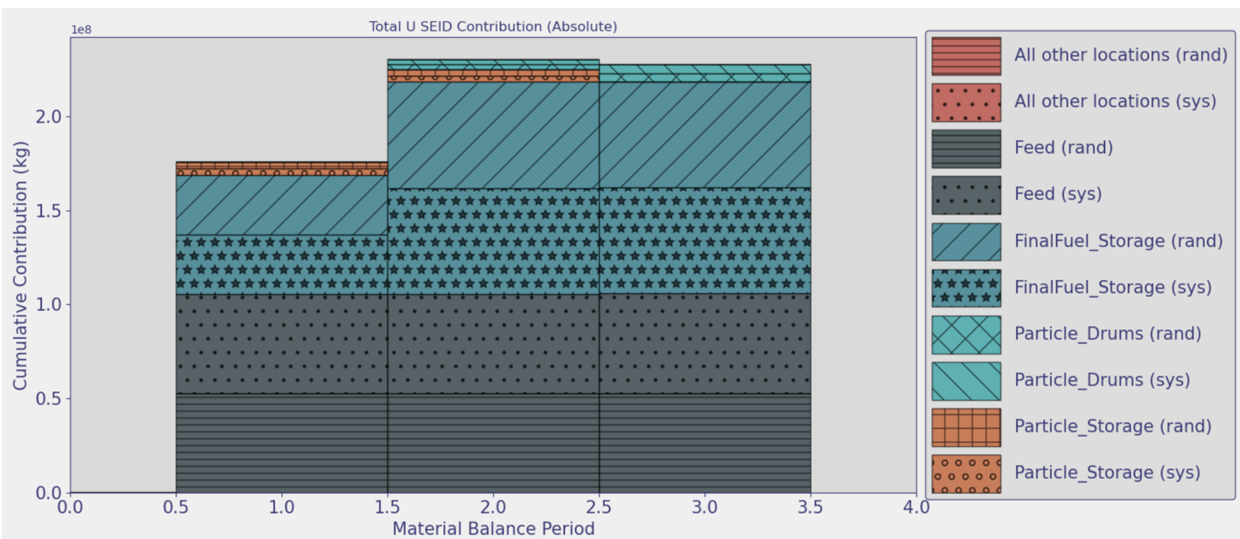

Figure 3-13. MAPIT results for measurement point contributions to standard error of the inventory difference for the generic TRISO fuel fabrication F3M model, with an MBP of 17,400 hours and random and systematic uncertainties at every KMP set to 1%.

Comparison of these results with NRC Category II requirements listed in Table 3-2 and the control limits on ID from DOE-STD-1194-2019 [19] give the following conclusions:

- The ID fluctuations are bounded by ±15,000 kg U (2250 kg of ^{235}U); the U ID is less than 3*SEID (~3*15,000 kg U = 45,000 kg U), but 2250 kg ^{235}U is greater than 9000 g (9 kg) of ^{235}U, so this result would require an investigation under NRC Category II thresholds.
- Setting all random and systematic uncertainties to 1% results in maintaining an SEID that is slightly higher than 2% of the active inventory. This does not meet the requirements of DOE Category I and II facilities per DOE-STD-1194-2019 [19], nor the investigate and report threshold of an NRC Category II facility (SEID<0.125% of active inventory).

However, as noted earlier, a fuel fabrication facility's SNM would likely be assigned an attractiveness level of E, and the facility would be assigned a categorization of IV.

Note that these results are based on setting all random and systematic uncertainties at all measurement points in Figure 2-2 and Figure 2-3 to 1%. This may not be a viable option, as 1) currently available measurement techniques for TRISO fuel fabrication facilities may not meet this uncertainty threshold, and 2) even if these measurement techniques are available, the process may be too expensive from a financial or efficiency perspective (or both).

4. SUMMARY AND FUTURE WORK

MC&A modeling efforts in FY25 focused on the development of a generic TRISO fuel fabrication facility model using the Fissile Facility Flow Modeler Simulink framework that improves upon previous modeling efforts by establishing a framework for representing the entire TRISO fuel fabrication process. The generic structure of the model allows for adaptability to any type of final TRISO fuel form, whether this form is spherical pebbles or cylindrical compacts, based on representing the chemical processes associated with the conversion of uranium feed into fuel. The outputs from the generic TRISO fuel fabrication F3M model have successfully been demonstrated to be implementable in the Material Accountancy Performance Indicator Toolkit software. This allows for statistical test analyses capable of showing how TRISO fuel fabrication facilities meet regulatory MC&A requirements.

4.1. Industry Engagement

The MPACT program is emphasizing industry engagement to promote collaboration between MPACT's MC&A technical experts and stakeholders in the DOE complex as well as industry aiming to develop MC&A plans for their fuel cycle facilities that meet regulatory requirements. In FY25, SNL began providing its MC&A modeling expertise to assist LANL with developing their MC&A plan for LEFFF. LANL plans to stand up LEFFF as a platform for TRISO fuel fabrication R&D and is currently collaborating with Kairos Power, Texas A&M University, and SNL within the Safeguards, Security and Accounting for Fuel Fabrication, Engineering, and Research (SSAFFER) working group. Kairos Power signed an agreement with LANL to become the first customer for LEFFF – the goal is to produce HALEU TRISO pebbles for Kairos Power's Hermes demonstration reactor series [21], [22].

LANL plans to stand up LEFFF for fuel production in 2026. As part of meeting LANL's requirements for establishing this facility, an MC&A plan for LEFFF must be approved by LANL's SAFE-NMCA organization. Details on the status of this task can be found in a separate report [23]. SNL plans to support LANL's development of the LEFFF MC&A plan via development of a LEFFF-specific F3M model, to be analyzed using MAPIT. The modeling effort will serve to provide statistical analyses capable of demonstrating the effect that proposed key measurement points, the measurement techniques that are planned for use, and their associated uncertainties have on calculations of ID, SEID, and statistical tests that demonstrate compliance with control limits as described in Section 3.1. These analyses are planned to contribute to optimization efforts for the LEFFF facility that simultaneously meet DOE Order 474.2A MC&A requirements and maximize production efficiencies. Optimizations are expected to be developed through determining the minimum necessary number of measurement points as well as the least intrusive measurement techniques that still satisfy regulatory requirements.

4.2. Suggested Model Improvements

Moving forward, modeling framework improvements will be iterative to address facility-specific needs. This iterative approach will serve as a demonstration of how the MPACT program's modeling tools and expertise can be leveraged to support MC&A needs for TRISO fuel fabrication facilities.

As mentioned in the LEFFF FY25 status update report [23], improvements to the F3M/MAPIT framework to support LEFFF will include the following considerations:

1. Accurate representation of LEFFF material throughput as a function of both quantity and time.
2. Expansion of the generic TRISO F3M modeling framework to conduct statistical tests for multiple MBAs.
3. Implementation of planned measurement techniques and their associated uncertainties. This will require an uncertainty analysis that converts manufacturer-specified instrument uncertainties into the random and systematic uncertainties that MAPIT uses for its statistical tests.
4. An MBP choice based on DOE Order 474.2A required physical inventory periods [18], which for Category IV quantities of SNM is 2 years for a processing MBA and 2 years for a storage MBA.

In addition, generally some assumptions were made about certain processes in the generic TRISO F3M model, including the treatment of final fuel form manufacturing process steps as simple time delays. The modeling framework can be developed via further investigation into pebble and compact processing steps for more accurate representation of these processes, as the addition of non-nuclear material surrounding the UCO kernels will impact the mass fraction of uranium within the materials that are inventoried at those final TRISO fuel form processing locations. However, a simplified approach that does not require the addition of chemical formulas to the final TRISO fuel form manufacturing steps can be taken where the process steps remain represented as simple time delays, but the mass fraction consideration is covered by the associated uncertainties of measurement techniques deployed at the final TRISO fuel form processing locations.

4.3. Conclusion

With comprehensive F3M/MAPIT functionality successfully demonstrated, the generic F3M TRISO fuel fabrication model can now be modified to represent actual TRISO fuel fabrication facilities, thus demonstrating its value to stakeholders such as DOE entities and industry. This value lies in both the capability to demonstrate regulatory compliance and analyze the impact of proposed measurement techniques on MC&A statistical tests to optimize facility efficiency and minimize the burden of MC&A requirements on facility operations.

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APPENDIX A. GENERIC TRISO FUEL FABRICATION F3M MODEL GUIDE

This Appendix is meant to serve as a guide for utilizing the TRISO fuel fabrication F3M model developed in FY25. The Appendix will have a breakdown of each variable, what each variable represents, the variable value or formula, and the variable units.

A.1. Material Balance Area 1: HALEU UO_2 Shipper/Receiver Area (Feed Generation and Interim Storage)

As noted in Section 2.1.1, MBA 1 in the TRISO fuel fabrication F3M model includes the interim storage area for HALEU UO_2 feed storage prior to sending drums of feed into MBA 2 for processing. Figure A-1 shows the section of the F3M model pertaining to the feed interim storage; Table A-1 and Table A-2 show the input variables and parameters for the HALEU UO_2 feed (custom source generator) block, while Table A-3 shows the parameters for the feed interim storage (entity hold (level)) block.

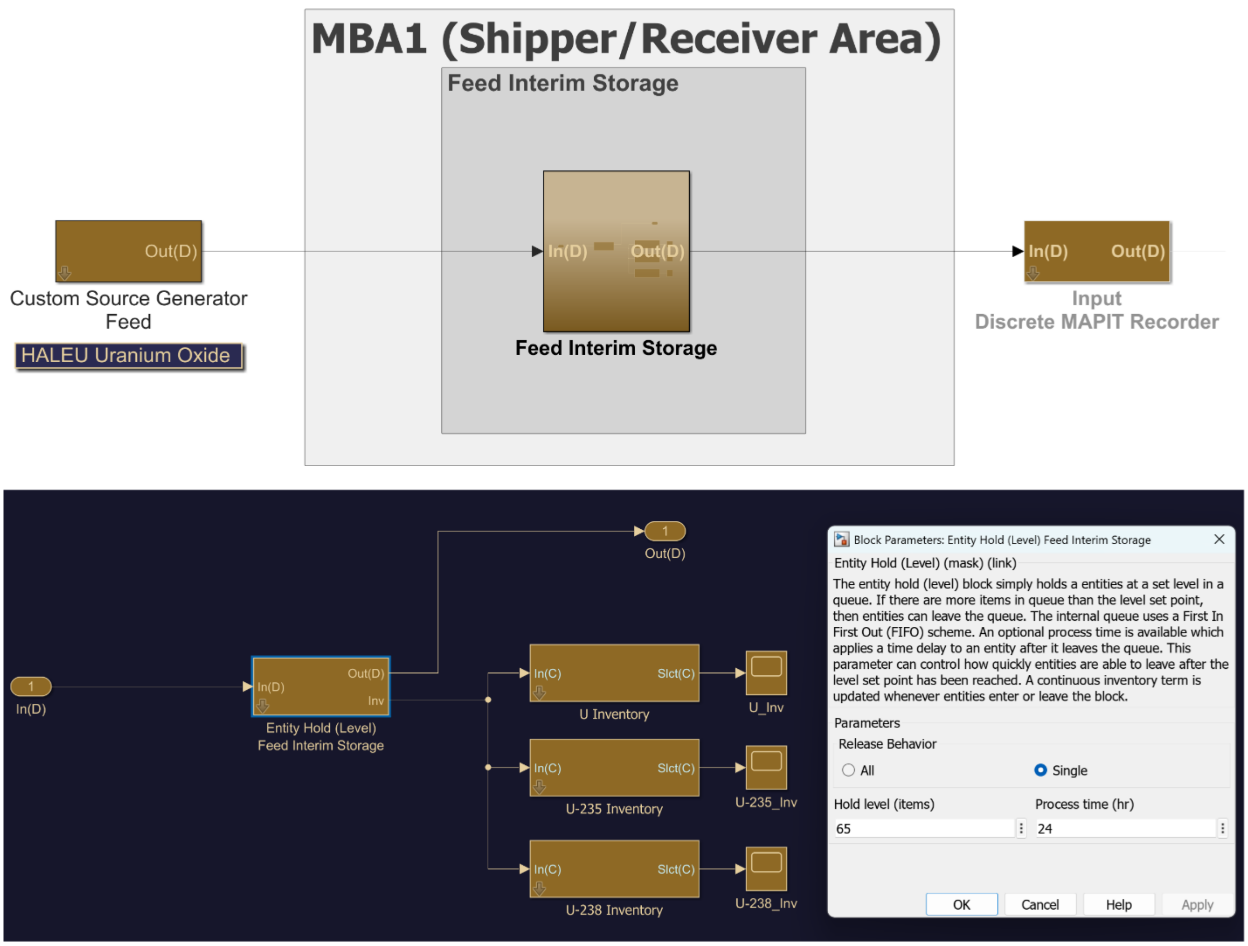

Figure A-1. HALEU UO_2 feed generation and interim storage section of the TRISO fuel fabrication F3M model.

Table A-1. HALEU UO_2 feed input variables.

Parameter	F3M Variable	Specified Value for Generic Model	Units
Drum size	$feedDrumSize$	1000	kg
Molar mass uranium	MMS_U	238	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Enrichment	$inputEnrichmentU235$	0.15	--
Operational days	$operationalDays$	300	days
Facility throughput	$throughput$	300	MTU/year

Table A-2. HALEU UO_2 feed parameters.

Parameter	F3M Variable	Value	Units
Molar mass UO_2	MMS_{UO_2}	$MMS_U + 2MMS_O$	kg/mol
^{235}U mass fraction	$fracU235$	$\frac{MMS_U * Input\ EnrichmentU235}{MMS_{UO_2}}$	--
^{238}U mass fraction	$fracU238$	$\frac{MMS_U(1 - Input\ EnrichmentU235)}{MMS_{UO_2}}$	--
O mass fraction	$fracO$	$1 - \left(\frac{MMS_U}{MMS_{UO_2}}\right)$	--
U per drum	$drumU$	$(fracU235 + fracU238) * feedDrumSize$	kg/year
Operational hours	$opHours$	$operationalDays * 24$	hr
1/throughput years (used to calculate drum period)	$drumYears$	$throughput * 1000/drumU$	years
Drum period	$drumPeriod$	$1/\left(\frac{drumYears}{opHours}\right)$	hr

Table A-3. Feed interim storage block parameters.

Parameter	Specified Value for Generic Model	Units
Hold level	65	Items (drums UO_2)
Process time	24	hr

A.2. Material Balance Area 2: TRISO Fuel Processing Area

A.2.1. Sub-MBA: UCO kernel manufacturing

This section includes descriptions of the blocks in the UCO kernel manufacturing sub-MBA within MBA 2 of the TRISO fuel fabrication F3M model.

A.2.1.1 Uranyl nitrate broth preparation

As noted in Section 2.1.2.1, the first process step in MBA 2 is the preparation of the uranyl nitrate block. Figure A-2 shows the section of the TRISO fuel fabrication F3M model corresponding to uranyl nitrate broth preparation; Table A-4 shows the input variables for the broth preparation block, while Table A-5 and Table A-6 show the parameters associated with the dissolution and hydrolysis steps, respectively.

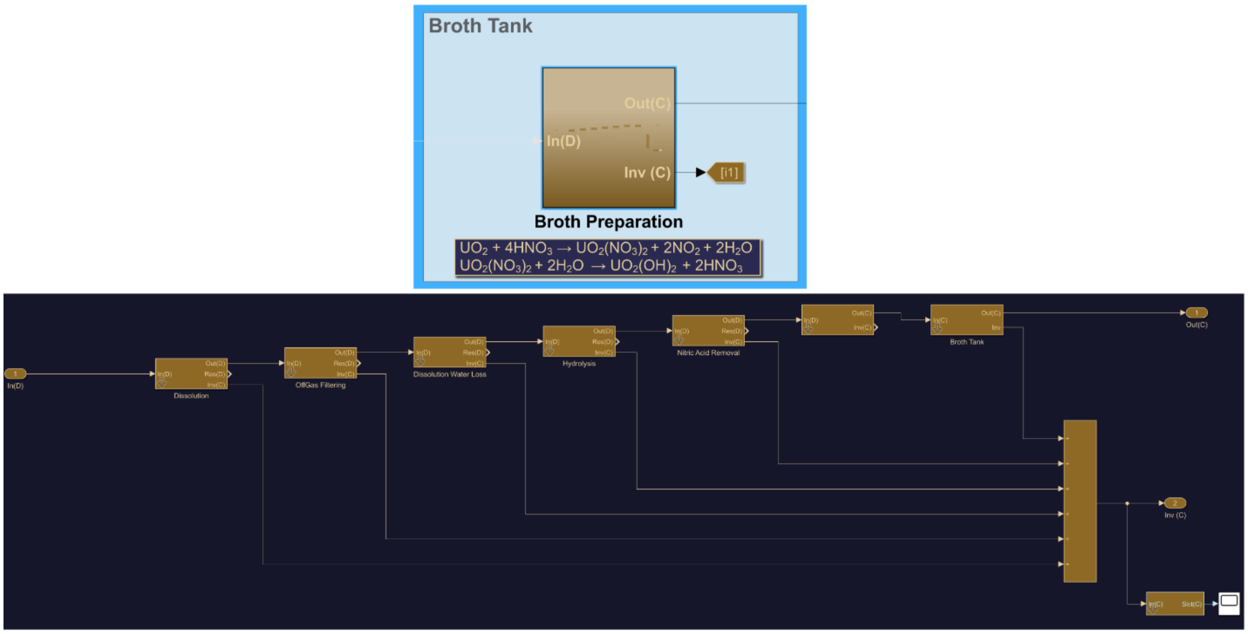

Figure A-2. Uranyl nitrate broth preparation section of the TRISO fuel fabrication F3M model.

Table A-4. Uranyl nitrate broth preparation input variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass hydrogen	MMS_H	1	kg/mol
Molar mass nitrogen	MMS_N	14	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-5. Uranyl nitrate broth preparation dissolution step variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass HNO_3	MMS_{HNO_3}	$MMS_H + MMS_N + 3MMS_O$	kg/mol
Molar mass $UO_2(NO_3)_2$	$MMS_{UO_2(NO_3)_2}$	$MMS_U + 2MMS_O + 2(MMS_N + 3MMS_O)$	kg/mol
Molar mass NO_2	MMS_{NO_2}	$MMS_N + 2MMS_O$	kg/mol
Molar mass H_2O	MMS_{H_2O}	$2MMS_H + MMS_O$	kg/mol
Dissolution			
Moles of UO_2 added to broth	$broth\_molUO2In$	$\frac{feedDrumSize}{MMS_{UO_2}}$	mol
Mass of nitric acid	$broth\_nitricAdd$	$4broth\_molUO2In * MMS_{HNO_3}$	kg
Hydrogen component of nitric acid addition block	$broth\_nitricH$	$\left(\frac{MMS_H}{MMS_{HNO_3}}\right)broth\_nitricAdd$	kg
Nitrogen component of nitric acid addition block	$broth\_nitricN$	$\left(\frac{MMS_N}{MMS_{HNO_3}}\right)broth\_nitricAdd$	kg
Oxygen component of nitric acid addition block	$broth\_nitricO$	$broth\_nitricAdd - broth\_nitricN - broth\_$	kg
Product of UO_2 dissolution in nitric acid	$broth\_dissolutionOutMass$	$broth\_molUO2In * MMS_{UO_2} + broth\_nitric$	kg
Off Gas Filtering			
Dissolution off gas filter mass	$broth\_dissGasFilterMass$	$broth\_dissolutionOutMass * \Big(\frac{}{MMS_{UO_2(NO_3}}$	kg
Nitrogen off gas	$broth\_offGasN$	$broth\_dissGasFilterMass\left(\frac{MMS_N}{MMS_{NO_2}}\right)$	kg
Oxygen off gas	$broth\_offGasO$	$broth\_dissGasFilterMass - broth\_offGas$	kg
Dissolution Water Loss			
Hydrogen from water lost in dissolution step (10% inefficiency)	$broth\_dissolutionHLoss$	$0.1broth\_dissolutionOutWater\left(\frac{2MMS_H}{MMS_{H_2O}}\right)$	kg
Oxygen from water lost in dissolution step (10% inefficiency)	$broth\_dissolutionOLoss$	$0.1broth\_dissolutionOutWater\left(\frac{MMS_O}{MMS_{H_2O}}\right)$	kg

Table A-6. Uranyl nitrate broth preparation hydrolysis step variables.

Parameter	F3M Variable	Value/Formula	Units
Hydrolysis			
Mass of uranyl nitrate input into hydrolysis	$broth\_uranylHydroInput$	$broth\_dissolutionOutMass * \left(\frac{M}{MMS_{UO_2(NO_3)_2}}\right.$	kg
Moles of uranyl nitrate input into hydrolysis	$broth\_uranylHydroMols$	$\frac{broth\_uranylHydroInput}{MMS_{UO_2(NO_3)_2}}$	mol
Water supplied from dissolution step	$broth\_dissolutionOutWater$	$broth\_uranylHydroMols * 2MMS_{H_2O}$	kg
Water needed for hydrolysis	$broth\_hydroWaterIn$	$2broth\_uranylHydroMols * MMS_{H_2O}$	kg
Additional water added to complete hydrolysis	$broth\_hydroWaterAdd$	$broth\_hydroWaterIn - 0.9broth\_dissolution$	kg
Hydrogen added to complete hydrolysis	$broth\_hydroH$	$broth\_hydroWaterAdd\left(\frac{2MMS_H}{MMS_{H_2O}}\right)$	kg
Oxygen added to complete hydrolysis	$broth\_hydroO$	$broth\_hydroWaterAdd - broth\_hydroH$	kg
Total mass of uranyl nitrate and water for hydrolysis	$broth\_hydroMassIn$	$broth\_uranylHydroInput + broth\_hydroWa$	kg
Nitric Acid Removal			
Hydrogen component of $2HNO_3$	$broth\_outHydroxH$	$\left(\frac{MMS_H}{MMS_{HNO_3}}\right)broth\_nitroHydroxOut$	kg
Nitrogen component of $2HNO_3$	$broth\_outHydroxN$	$\left(\frac{MMS_N}{MMS_{HNO_3}}\right)broth\_nitroHydroxOut$	kg
Oxygen component of $2HNO_3$	$broth\_outHydroxO$	$broth\_nitroHydroxOut - broth\_outHydroxH$	kg
$2HNO_3$ hydrolysis product	$broth\_nitroHydroxOut$	$broth\_hydroMassIn - broth\_uHydroxOut$	kg
Broth Tank			
Hydrogen component of $UO_2(OH_2)$	$broth\_outUranylH$	$\frac{2MMS_H}{MMS_{UO_2(OH)_2} * broth\_uHydroxOut}$	kg

Parameter	F3M Variable	Value/Formula	Units
Oxygen component of $UO_2(OH_2)$	$broth\_outUranylO$	$\frac{4MMS_O}{MMS_{UO_2(OH)_2} * broth\_uHydroxOut}$	kg
$UO_2(OH_2)$ hydrolysis product	$broth\_uHydroxOut$, $broth\_finalOutSize$	$broth\_hydroMassIn \left(\frac{MMS_{UO_2(OH)_2}}{MMS_{UO_2(OH)_2} + 2 \cdot MMS_{HNO_3}}\right)$	kg
Flow rate of $UO_2(OH_2)$ out to next process step	$broth\_outRate$	$\frac{broth\_finalOutSize}{drumPeriod}$	kg/hr

A.2.1.2 Kernel droplet formation and aging

As noted in Section 2.1.2.2, the uranyl nitrate is used to form kernel droplets, which are aged to convert from gelled to solid droplets. Figure A-3 shows the section of the TRISO fuel fabrication F3M model for kernel droplet formation & aging; Table A-7 shows the flow batcher block variables.

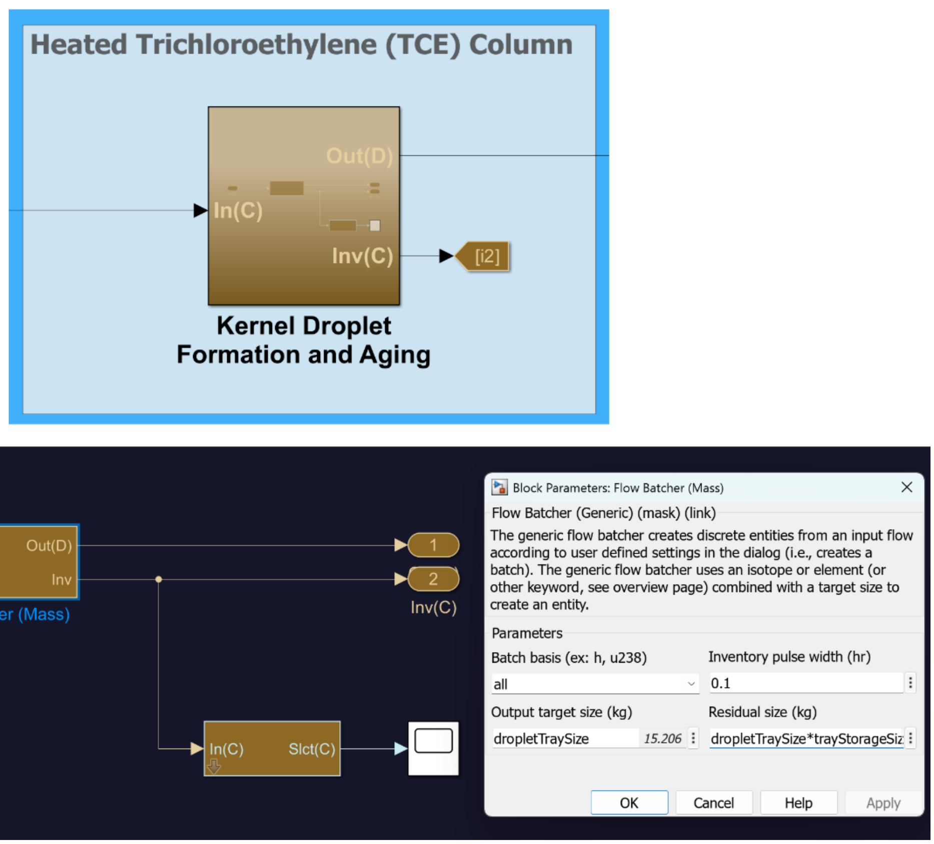

Figure A-3. Kernel droplet formation and aging section of the TRISO fuel fabrication F3M model.

Table A-7. Kernel droplet formation and aging block variables.

Parameter	F3M Variable	Formula	Units
Solid droplet tray size	*dropletTraySize*	$\frac{broth\_outRate}{3.5}$	kg
Tray storage size (mass of droplets in inventory)	*trayStorageSize*	$dropletTraySize * 10$	kg

A.2.1.3 Kernel washing and drying

As noted in Section 2.1.2.3, no chemical changes are expected for the kernel washing or drying steps. Therefore, these steps are modeled as simple time delays. Figure A-4 shows the washing/drying section of the TRISO fuel fabrication F3M model; Table A-8 shows the block parameters for kernel washing and drying.

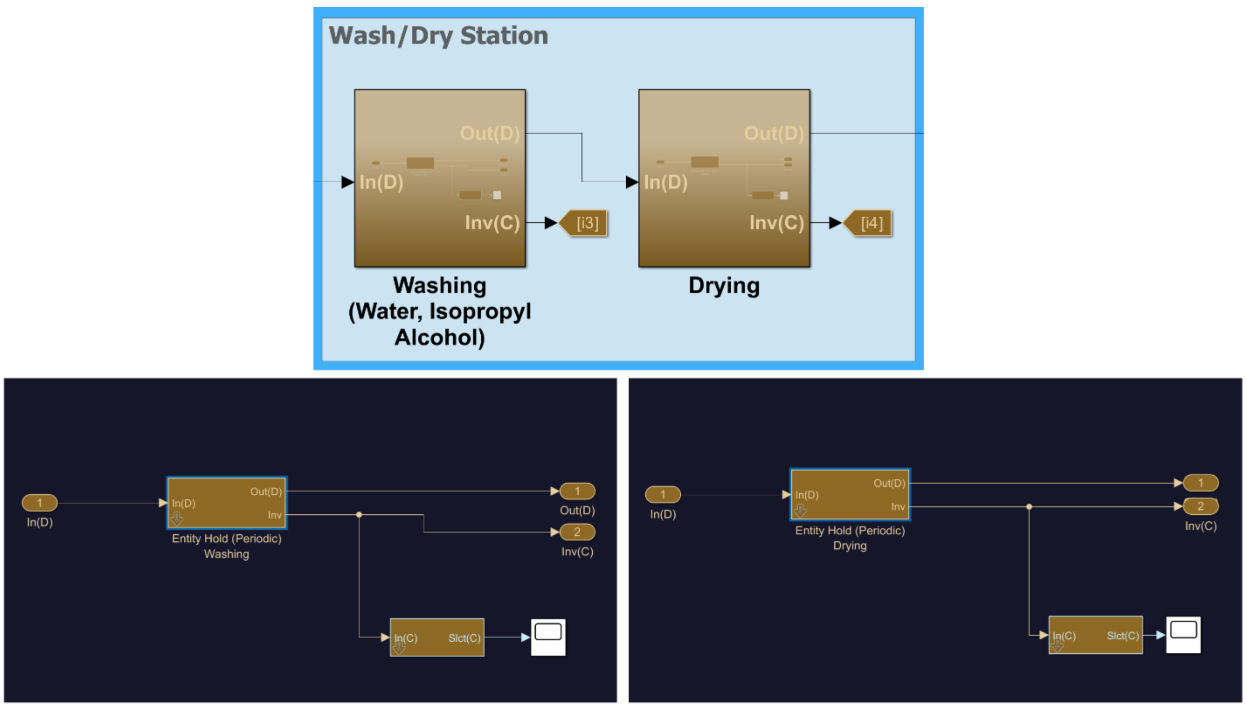

Figure A-4. Kernel washing and drying section of the TRISO fuel fabrication F3M model.

Table A-8. Kernel droplet washing block and drying block variables.

Parameter	Specified Value in Generic Model	Units
Washing process time	24	hr
Drying process time	24	hr

A.2.1.4 Kernel calcination

As noted in Section 2.1.2.4, the calcination steps simulated in the TRISO fuel fabrication F3M model are based on a UO_2 feed and therefore take an input of uranyl nitrate, rather than ADU as indicated in IAEA-TECDOC-1645 [3]. Figure A-5 shows the section of the model representing the calcination step; Table A-9 and Table A-10 show the variables associated with the calcination process modeled in F3M.

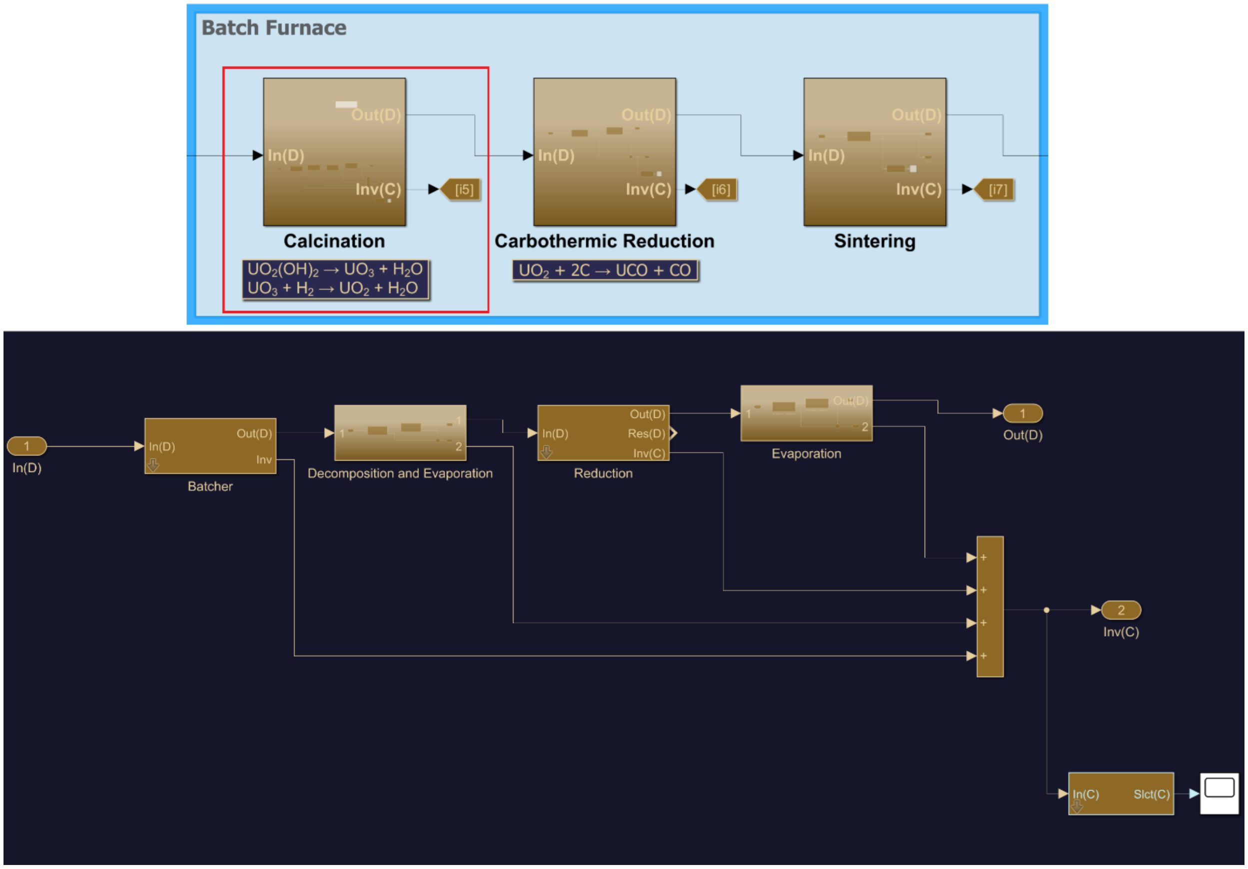

Figure A-5. Kernel calcination section of the TRISO fuel fabrication F3M model.

Table A-9. Kernel calcination input variables.

Parameter	F3M Variable	Value	Units
Molar mass hydrogen	MMS_H	1	kg/mol
Molar mass nitrogen	MMS_N	14	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-10. Kernel calcination process variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass $UO_2(OH)_2$	$MMS_{UO_2(OH)_2}$	$MMS_U + 2MMS_O + 2(MMS_O + MMS_H)$	kg/mol
Molar mass UO_3	MMS_{UO_3}	$MMS_U + 3MMS_O$	kg/mol
Molar mass H_2O	MMS_{H_2O}	$2MMS_H + MMS_O$	kg/mol
Molar mass UO_2	MMS_{UO_2}	$MMS_U + 2MMS_O$	kg/mol

Batcher			
Calcination batch size	$calc\_batchSize$	$dropletTraySize * trayStorageSize$	kg
Mass of $UO_2(OH)_2$ undergoing calcination	$calcIn$	$calc\_batchSize$	kg
Moles of $UO_2(OH)_2$ undergoing calcination	$calc\_molIn$	$\frac{calcIn}{MMS_{UO_2(OH)_2}}$	mol
Batch threshold (sum of all elements/isotopes by mass)	Unspecified variable (constant)	149.9	kg
Decomposition and Evaporation			
UO_3 product from calcination	$calc\_UO3Out$	$calc\_molIn * MMS_{UO_3}$	kg
H_2O product from calcination	$calc\_water1Out$	$calcIn - calc\_UO3Out$	kg
Hydrogen removed via water evaporation prior to reduction step	$calc\_water1HOut$ (variable not directly used in model; H removed using multiplicative block instead)	$calc\_water1Out * \left(\frac{2 * MMS_H}{MMS_{H_2O}}\right)$	kg
Oxygen removed via water evaporation prior to reduction step	$calc\_water1OOut$	$calc\_water1Out - calc\_water1HOut$	kg
Reduction			
UO_3 undergoing reduction	$calc\_UO3In$	$calc\_molIn * MMS_{UO_3}$	kg
H_2 added for reduction	$calc\_HAdd$	$calc\_molIn * 2MMS_H$	kg
H_2O product from reduction	$calc\_water2Out$	$(calc\_UO3In + calc\_Hadd) - calc\_UO2Out$	kg
UO_2 product from reduction (output from calcination block moving into next process step)	$calc\_UO2Out$; $calc\_finalOut$	$(calc\_UO3In + calc\_HAdd) * \left(\frac{MMS_{U}}{MMS_{UO_2} + M}\right.$	kg
Evaporation			
Hydrogen removed via evaporation of water from reduction	$calc\_water2HOut$ (variable not directly used in model; H removed using multiplicative block instead)	$calc\_water2Out * \left(\frac{2MMS_H}{MMS_{H_2O}}\right)$	kg
Oxygen removed via evaporation of water from reduction	$calc\_water2OOut$	$calc\_water2Out - calc\_water2HOut$	kg

A.2.1.5 Kernel carbothermic reduction

As noted in Section 2.1.2.5, the UO_2 kernels undergo carbothermic reduction to produce UCO with a carbon monoxide byproduct. Figure A-6 shows the carbothermic reduction section of the TRISO fuel fabrication F3M model; the parameters are shown in Table A-11 and Table A-12.

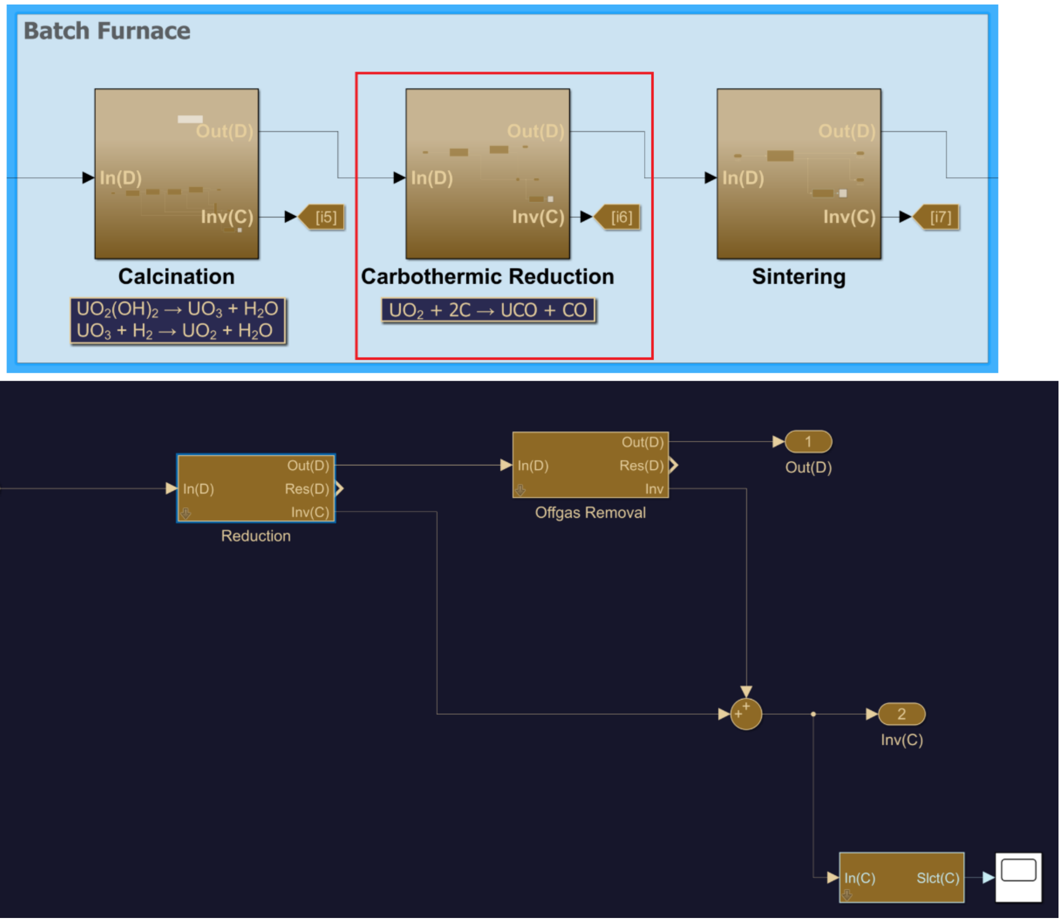

Figure A-6. Kernel carbothermic reduction section of the TRISO fuel fabrication F3M model.

Table A-11. Kernel carbothermic reduction input variables.

Parameter	F3M Variable	Value	Units
Molar mass carbon	MMS_C	12	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-12. Kernel carbothermic reduction process variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass UO_2	MMS_{UO_2}	$MMS_U + 2MMS_O$	kg/mol
Molar mass UCO	MMS_{UCO}	$MMS_U + MMS_C + MMS_O$	kg/mol
Molar mass CO	MMS_{CO}	$MMS_C + MMS_O$	kg/mol

Reduction			
UO_2 undergoing carbothermic reduction (following calcination)	$carbo\_In$	$calc\_finalOut$	kg
Mass of oxygen going into carbothermic reduction	$carbo\_omass$	$\frac{calc\_finalOut}{MMS_{UO_2} * \left(\frac{32}{MMS_{UO_2}}\right)}$	kg
Moles of UO_2 undergoing carbothermic reduction	$carbo\_molIn$	$\frac{carbo\_In}{MMS_{UO_2}}$	mol
Mass of carbon going into carbothermic reduction	$carbo\_cAdd$	$\frac{carbo\_molIn}{2MMS_C}$	kg
Mass of UCO product	$carbo\_UCOOut$; $carbo\_finalOut$	$carbo\_molIn * MMS_{UCO}$	kg
Mass of CO product	$carbo\_COOut$	$carbo\_molIn * MMS_{CO}$	kg
Off Gas Removal			
Fraction of carbon removed from CO off gas	$carbo\_cRemove$	0.5	--
Fraction of oxygen removed from CO off gas	$carbo\_oRemove$	0.5	--

A.2.1.6 Kernel sintering

As noted in Section 2.1.2.6, the kernels undergo sintering as a densification step. Since no chemical composition changes occur, the TRISO fuel fabrication F3M model simulates this step as a periodic entity hold. Figure A-7 shows the sintering section of the F3M model; the only parameter of interest (process time) is shown in Table A-13.

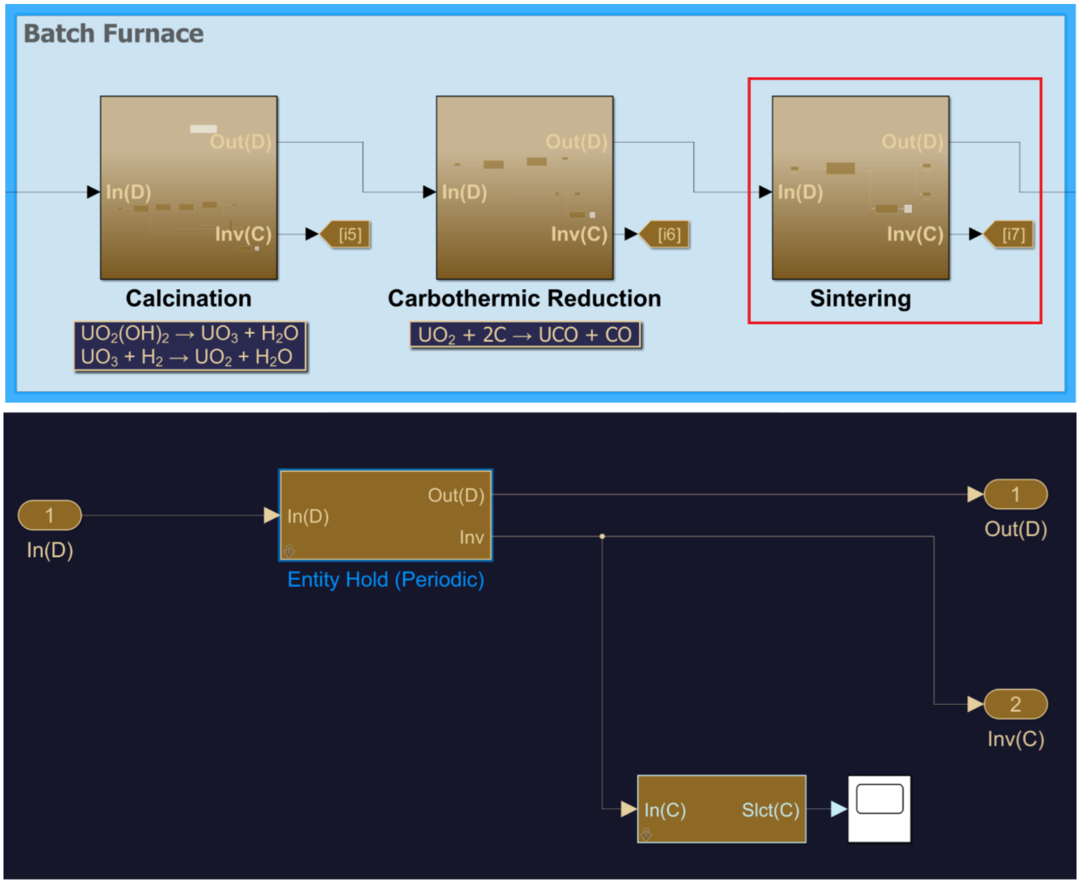

Figure A-7. Kernel sintering section of the TRISO fuel fabrication F3M model.

Table A-13. Kernel sintering process time in the TRISO fuel fabrication F3M model.

Parameter	Value	Units
Kernel sintering process time	24	hr

A.2.1.7 Kernel sieving and sorting

As noted in Section 2.1.2.7, the sintered kernels are sieved and sorted to select for uniform kernels; the non-uniform kernels are filtered out by the sieving table and are considered waste. Figure A-8 shows the sieving and sorting section of the TRISO fuel fabrication F3M model; the sieving model parameters are shown in Table A-14.

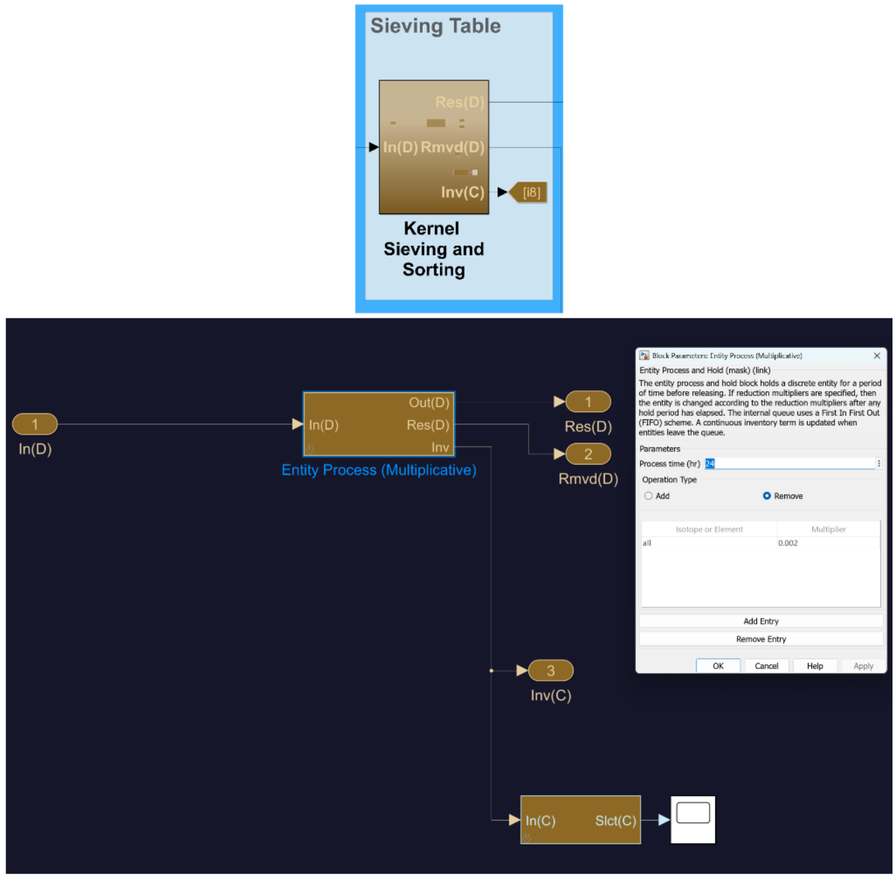

Figure A-8. Kernel sieving and sorting section of the TRISO fuel fabrication F3M model.

Table A-14. Kernel sieving and sorting parameters in the TRISO fuel fabrication F3M model.

Parameter	Value	Units
Process time	24	hr
Entity removal multiplicative factor (fraction of sintered kernels filtered out and sent to waste)	0.002	--

A.2.1.8 UCO kernel interim storage and drum packaging

As noted in Section 2.1.2.8, the product UCO kernels from the kernel manufacturing sub-MBA are modeled as being intermittently stored before packaged in drums to be moved to the next processing sub-MBA, where the kernels will undergo the buffer PyC, IPyC, SiC, and OPyC coating stages. Figure A-9 shows the interim storage and drum packaging sections of the TRISO fuel fabrication F3M model; Table A-15 shows the model parameters for the last portion of this sub-MBA.

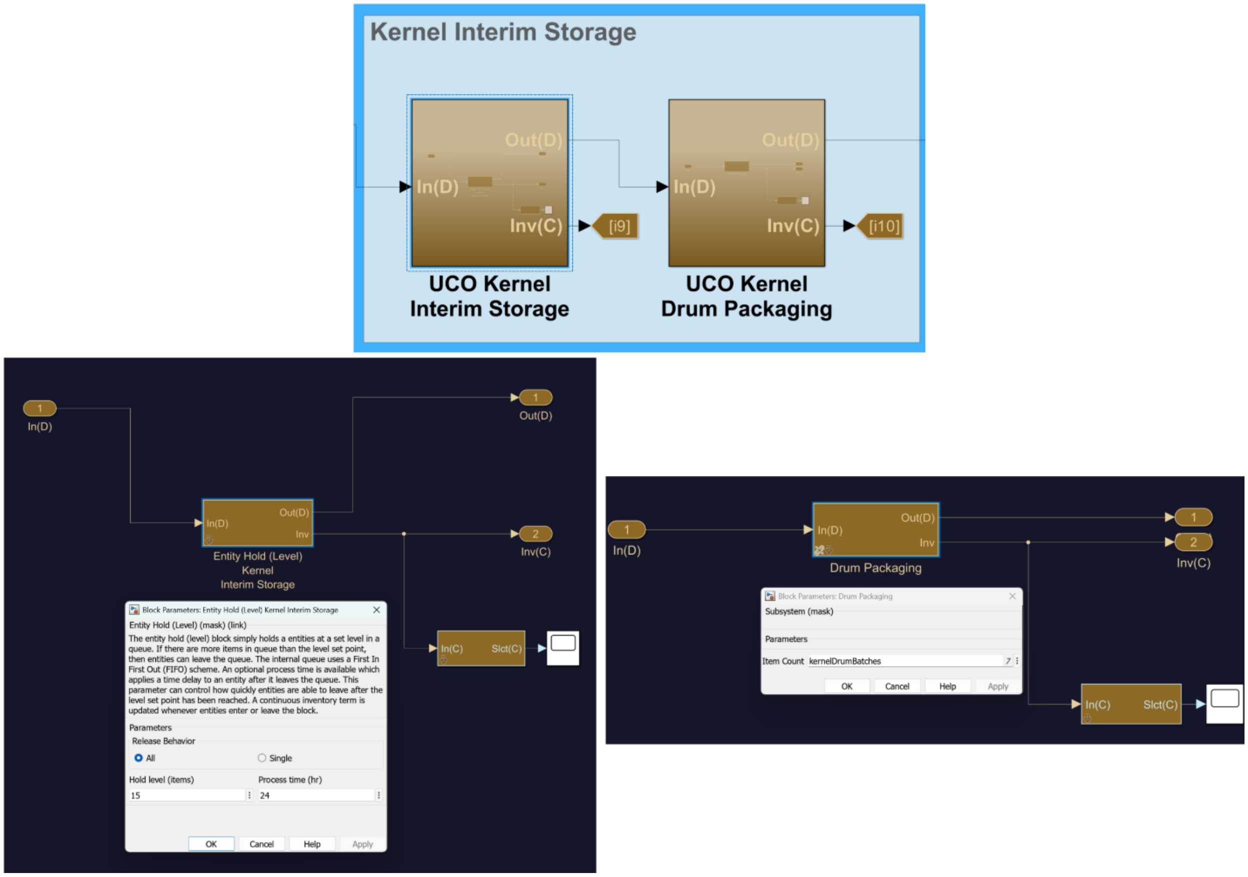

Figure A-9. Kernel interim storage and drum packaging section of the TRISO fuel fabrication F3M model.

Table A-15. Kernel interim storage and drum packaging parameters in the TRISO fuel fabrication F3M model.

Parameter	F3M Variable	Value	Units
Entity hold level	--	15	items
Interim storage process time	--	24	hr
Drum packaging batches	*kernelDrumBatches*	7	--

A.2.2. Sub-MBA: coated particle manufacturing

This section includes details on the coated particle manufacturing sub-MBA within the TRISO fuel fabrication F3M model.

A.2.2.1 PyC buffer layer deposition

As noted in Section 2.1.3.1, the UCO kernels are first coated with a PyC buffer layer via the decomposition of acetylene. Figure A-10 shows the PyC buffer layer deposition section of the TRISO fuel fabrication F3M model, while Table A-16 and Table A-17 show the parameters associated with this first coating layer.

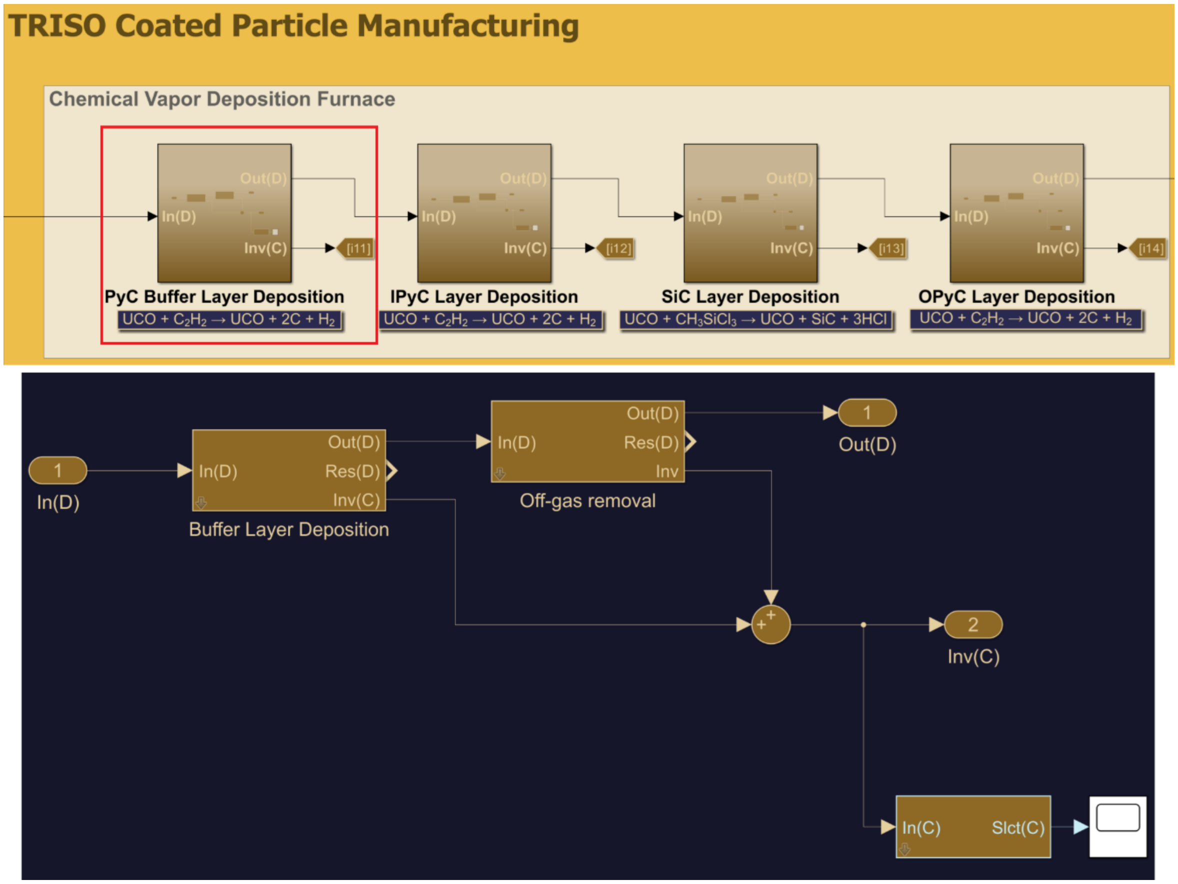

Figure A-10. PyC buffer layer deposition section of the TRISO fuel fabrication F3M model.

Table A-16. PyC buffer layer deposition input variables.

Parameter	F3M Variable	Value	Units
Molar mass hydrogen	MMS_H	1	kg/mol
Molar mass carbon	MMS_C	12	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-17. PyC buffer layer deposition process variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass UCO	MMS_{UCO}	$MMS_U + MMS_C + MMS_O$	kg/mol
Molar mass C_2H_2	$MMS_{C_2H_2}$	$2MMS_C + 2MMS_H$	kg/mol

Buffer Layer Deposition			
Mass of UCO kernels undergoing PyC buffer layer deposition	pyc_in	$kernelDrumBatches * carbo\_UCOOut$	kg
Moles of UCO kernels undergoing PyC buffer layer deposition	pyc_molUCO	$\frac{pyc\_in}{MMS_{UCO}}$	mol
Mass of C_2H_2 added for decomposition	$pyc\_c2h2add$	$\frac{pyc\_molUCO}{MMS_{C_2H_2}}$	kg
Mass of carbon added for decomposition	pyc_c2add	$pyc\_c2h2add * \left(\frac{2MMS_C}{MMS_{C_2H_2}}\right)$	kg
Mass of hydrogen added for decomposition	pyc_h2add	$pyc\_c2h2add - pyc\_c2add$	kg
Mass of UCO product	pyc_out	$pyc\_in + pyc\_c2add$	kg
Off Gas Removal			
Fraction of hydrogen removed from H_2 off gas	$pyc\_h2remove$ (variable not directly used in model; H removed using multiplicative block instead)	1	--

A.2.2.2 IPyC layer deposition

As noted in Section 2.1.3.2, the next coating layer following the PyC buffer layer is the IPyC layer. For simplicity, the TRISO fuel fabrication F3M modeling framework only includes the addition of acetylene for this process step, even though IAEA-TECDOC-1645 [3] also includes the addition of propylene. Figure A-11 shows the IPyC layer deposition section of the TRISO fuel fabrication F3M model, while Table A-18 and Table A-19 show the model parameters.

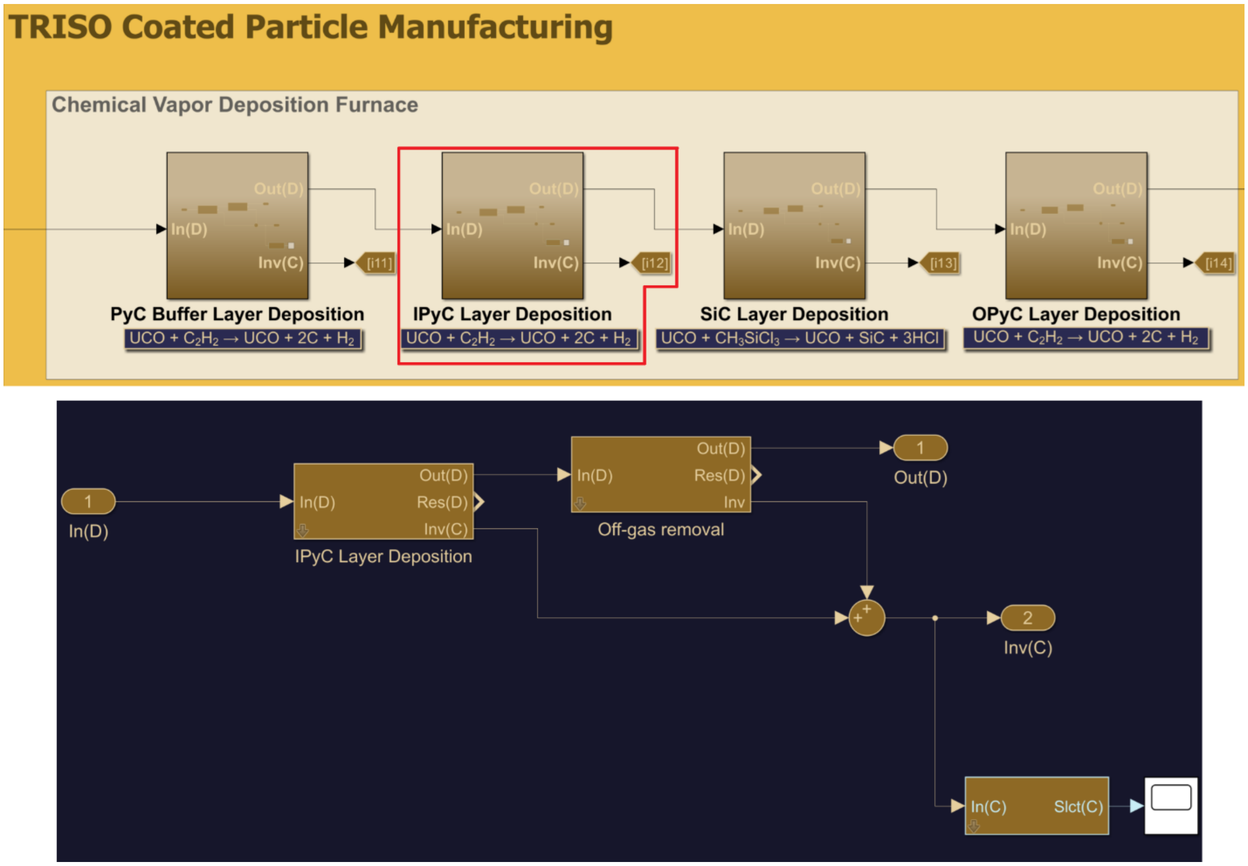

Figure A-11. IPyC layer deposition section of the TRISO fuel fabrication F3M model.

Table A-18. IPyC layer deposition input variables.

Parameter	F3M Variable	Value	Units
Molar mass hydrogen	MMS_H	1	kg/mol
Molar mass carbon	MMS_C	12	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-19. IPyC layer deposition process variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass UCO	MMS_{UCO}	$MMS_U + MMS_C + MMS_O$	kg/mol
Molar mass C_2H_2	$MMS_{C_2H_2}$	$2MMS_C + 2MMS_H$	kg/mol

IPyC Layer Deposition			
Mass of UCO kernels undergoing IPyC layer deposition	$ipyc\_in$	pyc_in	kg
Mass of C_2H_2 added for decomposition	$ipyc\_c2h2add$	$\left(\frac{ipyc\_in}{MMS_{UCO}}\right) * MMS_{C_2H_2}$	kg
Mass of carbon added for decomposition	$ipyc\_c2add$	$ipyc\_c2h2add * \left(\frac{2MMS_C}{MMS_{C_2H_2}}\right)$	kg
Mass of hydrogen added for decomposition	$ipyc\_h2add$	$ipyc\_c2h2add - ipyc\_c2add$	kg
Mass of IPyC-coated UCO kernel product	$ipyc\_out$	$pyc\_out + ipyc\_c2add$	kg
Off Gas Removal			
Fraction of hydrogen removed from H_2 off gas	$ipyc\_h2remove$ (variable not directly used in model; H removed using multiplicative block instead)	1	--

A.2.2.3 SiC layer deposition

As noted in Section 2.1.3.3, the SiC layer is deposited on top of the IPyC layer via decomposition of methyltrichlorosilane. Figure A-12 shows the SiC layer deposition section of the TRISO fuel fabrication F3M model, while Table A-20 and Table A-21 show the corresponding model parameters.

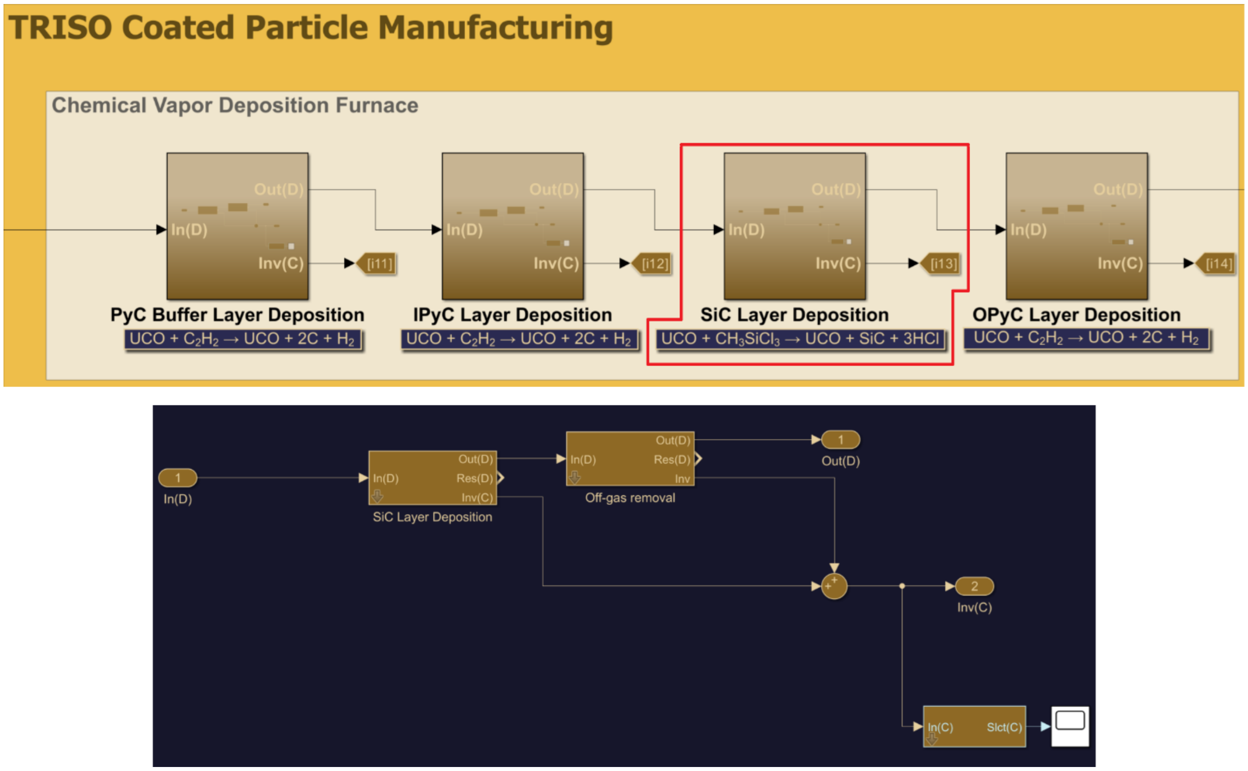

Figure A-12. SiC layer deposition section of the TRISO fuel fabrication F3M model.

Table A-20. SiC layer deposition input variables.

Parameter	F3M Variable	Value	Units
Molar mass hydrogen	MMS_H	1	kg/mol
Molar mass carbon	MMS_C	12	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass silicon	MMS_{Si}	28	kg/mol
Molar mass chlorine	MMS_{Cl}	35	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-21. SiC layer deposition process variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass UCO	MMS_{UCO}	$MMS_U + MMS_C + MMS_O$	kg/mol
Molar mass CH_3SiCl_3	$MMS_{CH_3SiCl_3}$	$MMS_C + 3MMS_H + MMS_{Si} + 3MMS_{Cl}$	kg/mol

SiC Layer Deposition			
Mass of UCO kernels undergoing SiC layer deposition	sic_in	pyc_in	kg
Mass of CH_3SiCl_3 added for decomposition	$sic\_ch3sicl3add$	$\left(\frac{ipyc\_in}{MMS_{UCO}}\right) * MMS_{CH_3SiCl_3}$	kg
Mass of carbon added for decomposition	sic_cadd	$sic\_ch3sicl3add * \left(\frac{MMS_C}{MMS_{CH_3SiCl_3}}\right)$	kg
Mass of hydrogen added for decomposition	sic_hadd	$sic\_ch3sicl3add * \left(\frac{3MMS_H}{MMS_{CH_3SiCl_3}}\right)$	kg
Mass of silicon added for decomposition	sic_siadd	$sic\_ch3sicl3add * \left(\frac{MMS_{Si}}{MMS_{CH_3SiCl_3}}\right)$	kg
Mass of chlorine added for decomposition	sic_cladd	$sic\_ch3sicl3add - (sic\_cadd + sic\_hadd +$	kg
Mass of UCO in SiC-coated kernel	sic_ucoOut	pyc_in	kg
Mass of SiC product	sic_sicOut	$sic\_siadd + sic\_cadd$	kg
Mass of HCl product	sic_hclOut	$sic\_hadd + sic\_cladd$	kg
Mass of SiC-coated UCO kernel product	sic_out	$ipyc\_out + sic\_sicOut$	kg
Off Gas Removal			
Fraction of hydrogen removed from HCl off gas	Unspecified variable	1	--
Fraction of chlorine removed from HCl off gas	Unspecified variable	1	--

A.2.2.4 OPyC layer deposition

As noted in Section 2.1.3.4, the final TRISO coating is the OPyC layer. For simplicity, the TRISO fuel fabrication F3M model assumes that this layer is formed via decomposition of acetylene. Figure A-13 shows the OPyC layer deposition section of the model; Table A-22 and Table A-23 show the model parameters.

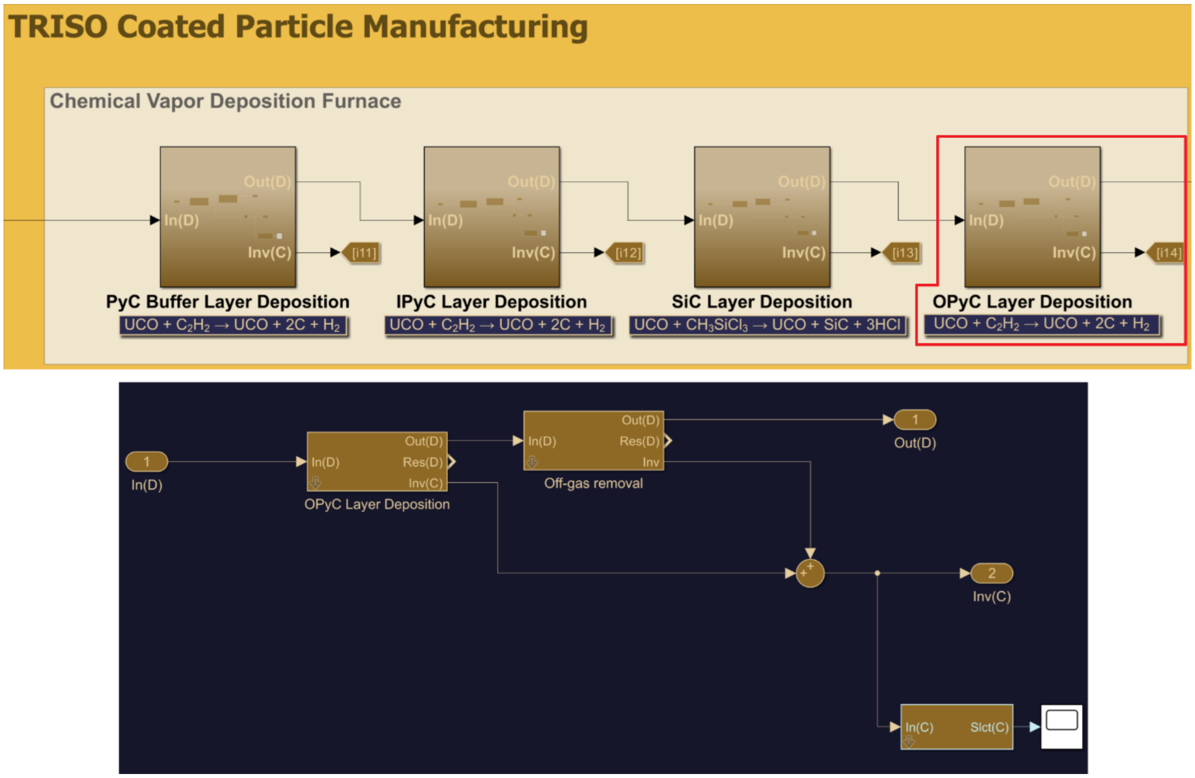

Figure A-13. OPyC layer deposition section of the TRISO fuel fabrication F3M model.

Table A-22. OPyC layer deposition input variables.

Parameter	F3M Variable	Value	Units
Molar mass hydrogen	MMS_H	1	kg/mol
Molar mass carbon	MMS_C	12	kg/mol
Molar mass oxygen	MMS_O	16	kg/mol
Molar mass silicon	MMS_{Si}	28	kg/mol
Molar mass chlorine	MMS_{Cl}	35	kg/mol
Molar mass uranium	MMS_U	238	kg/mol

Table A-23. OPyC layer deposition process variables.

Parameter	F3M Variable	Value/Formula	Units
Molar mass UCO	MMS_{UCO}	$MMS_U + MMS_C + MMS_O$	kg/mol
Molar mass C_2H_2	$MMS_{C_2H_2}$	$2MMS_C + 2MMS_H$	kg/mol

OPyC Layer Deposition			
Mass of UCO kernels undergoing OPyC layer deposition	$opyc\_in$	pyc_in	kg
Mass of C_2H_2 added for decomposition	$sic\_c2h2add$ (updated variable)	$\left(\frac{opyc\_in}{MMS_{UCO}}\right) * MMS_{C_2H_2}$	kg
Mass of carbon added for decomposition	sic_c2add (updated variable)	$sic\_c2h2add * \left(\frac{2MMS_C}{MMS_{C_2H_2}}\right)$	kg
Mass of hydrogen added for decomposition	sic_h2add (updated variable)	$sic\_c2h2add - sic\_c2add$	kg
Mass of SiC-coated UCO kernel product	sic_out (updated variable)	$sic\_out + sic\_c2add$	kg
Off Gas Removal			
Fraction of hydrogen removed from H_2 off gas	$sic\_h2remove$ (updated variable; variable not directly used in model; H removed using multiplicative block instead)	1	--

A.2.2.5 Coated particle sieving and sorting

As noted in Section 2.1.3.6, the coated TRISO particles are sieved and sorted to select for uniform particles; the non-uniform particles are filtered out by the sieving table and are considered waste. Figure A-14 shows the sieving and sorting section of the TRISO fuel fabrication F3M model; the sieving model parameters are shown in Table A-24.

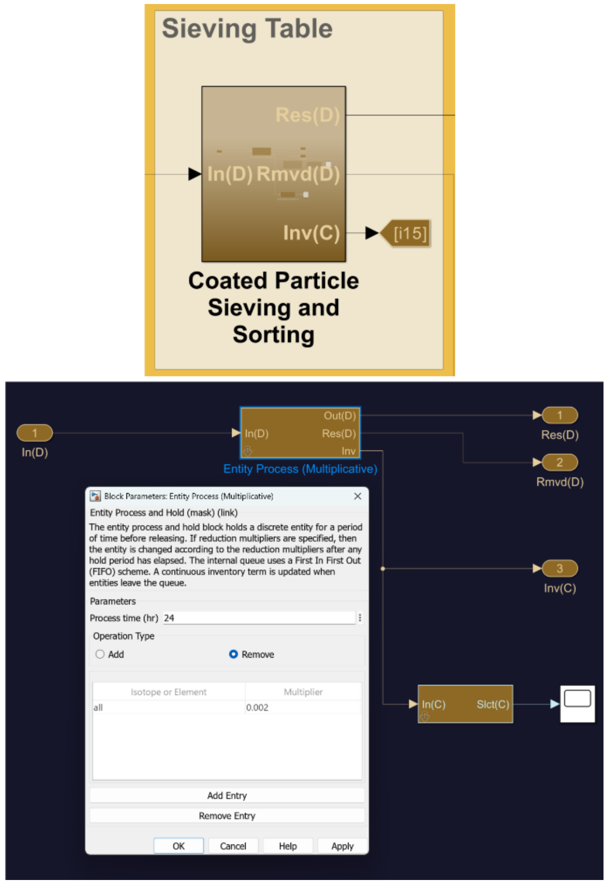

Figure A-14. Coated particle sieving and sorting section of the TRISO fuel fabrication F3M model.

Table A-24. Coated particle sieving and sorting parameters in the TRISO fuel fabrication F3M model.

Parameter	F3M Variable	Value	Units
Process time	*coatedSieveTime*	24	hr
Entity removal multiplicative factor (fraction of coated particles filtered out and sent to waste)	*coatedSieveLoss*	0.002	--

A.2.2.6 Coated particle interim storage and drum packaging

As noted in Section 2.1.3.6, drums of coated particles are intermittently stored prior to transfer to the final TRISO fuel form manufacturing sub-MBA. Figure A-15 shows the coated particle interim storage and drum packaging section of the TRISO fuel fabrication F3M model; Table A-25 shows the parameters associated with this storage and transfer.

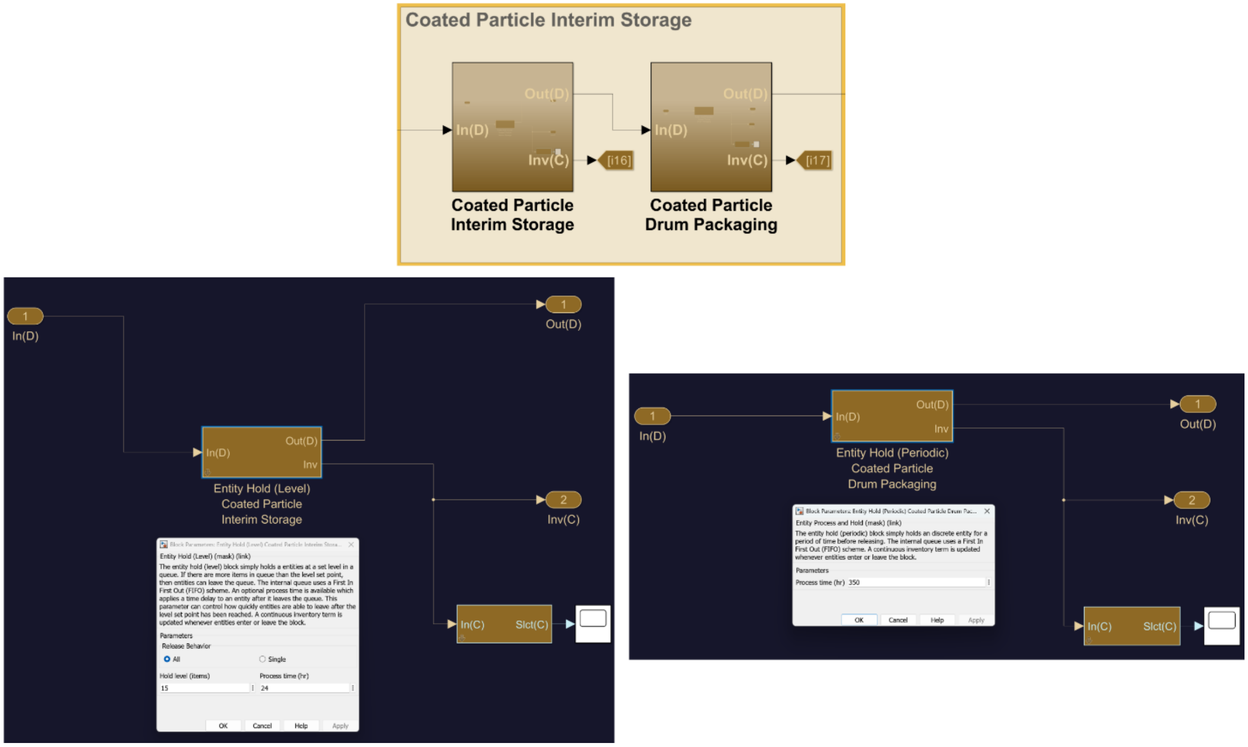

Figure A-15. Coated particle interim storage and drum packaging section of the TRISO fuel fabrication F3M model.

Table A-25. Coated particle interim storage and drum packaging parameters in the TRISO fuel fabrication F3M model.

Parameter	F3M Variable	Value	Units
Entity hold level	*particleStorageLevel*	15	items
Interim storage batch process time	*particleStorageTime*	24	hr
Particle drum packaging time	*particleDrumPackageTime*	350	hr

A.2.3. Sub-MBA: TRISO final fuel form manufacturing

This section includes details on the TRISO final fuel form manufacturing sub-MBA within the TRISO fuel fabrication F3M model.

A.2.3.1 Overcoating and warm pressing of TRISO particles

As noted in Section 2.1.4.1, the first step in manufacturing the final TRISO fuel form (spherical pebbles or cylindrical compacts) involves overcoating the TRISO coated particles with graphitic matrix material. Due to the lack of information on the chemical processes associated with overcoating as well as the mass fractions of TRISO coated particles and graphitic matrix material in IAEA-TECDOC-1645 [3], this process is modeled as a simple time delay. Figure A-16 shows the TRISO particle overcoating step in the F3M model; Table A-26 shows the time delay represented in the model.

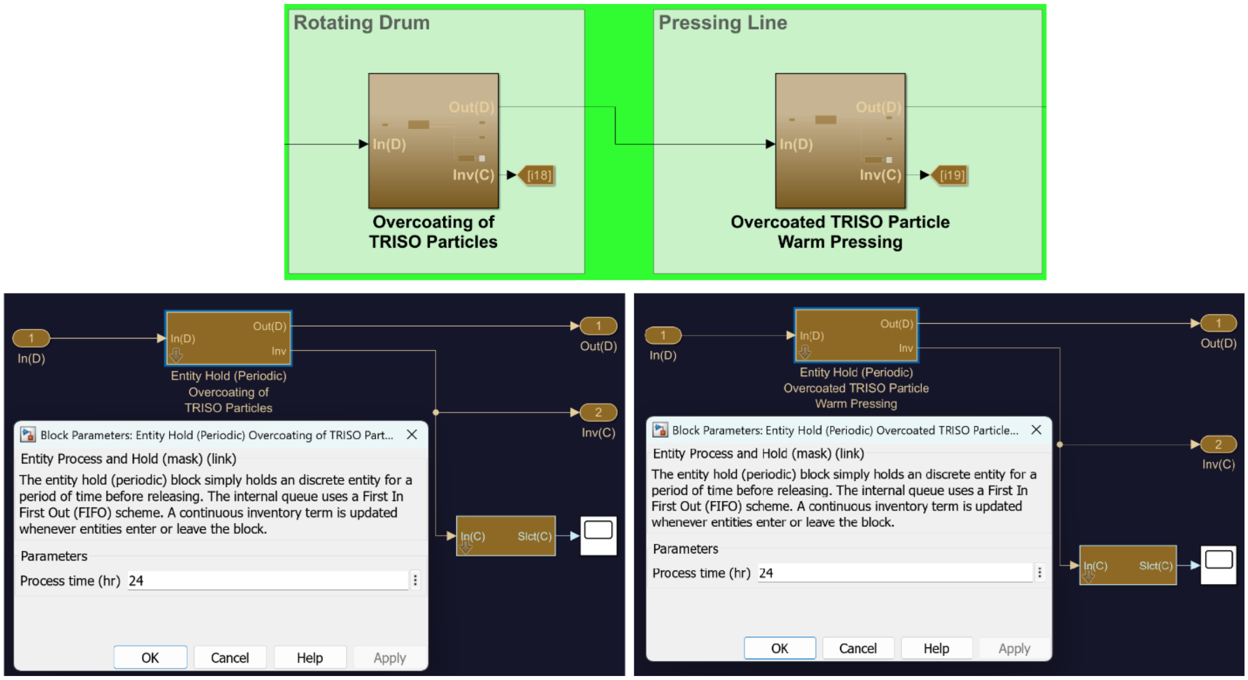

Figure A-16. TRISO particle overcoating and warm pressing sections of the TRISO fuel fabrication F3M model.

Table A-26. TRISO particle overcoating and warm pressing process times in the TRISO fuel fabrication F3M model.

Parameter	Value	Units
Overcoating process time	24	hr
Warm pressing process time	24	hr

A.2.3.2 Carbonization and annealing

As shown in Section 2.1.4.2, the warm pressed TRISO fuel is placed in a furnace, first to carbonize the phenolic resin binder, then to be annealed to remove impurities and de-gas the fuel. As with the other TRISO final fuel form manufacturing steps represented in this modeling framework, the carbonization and annealing steps are modeled as simple time delays. Figure A-17 shows the carbonization and annealing sections of the TRISO fuel fabrication F3M model; Table A-27 shows the carbonization and annealing process times.

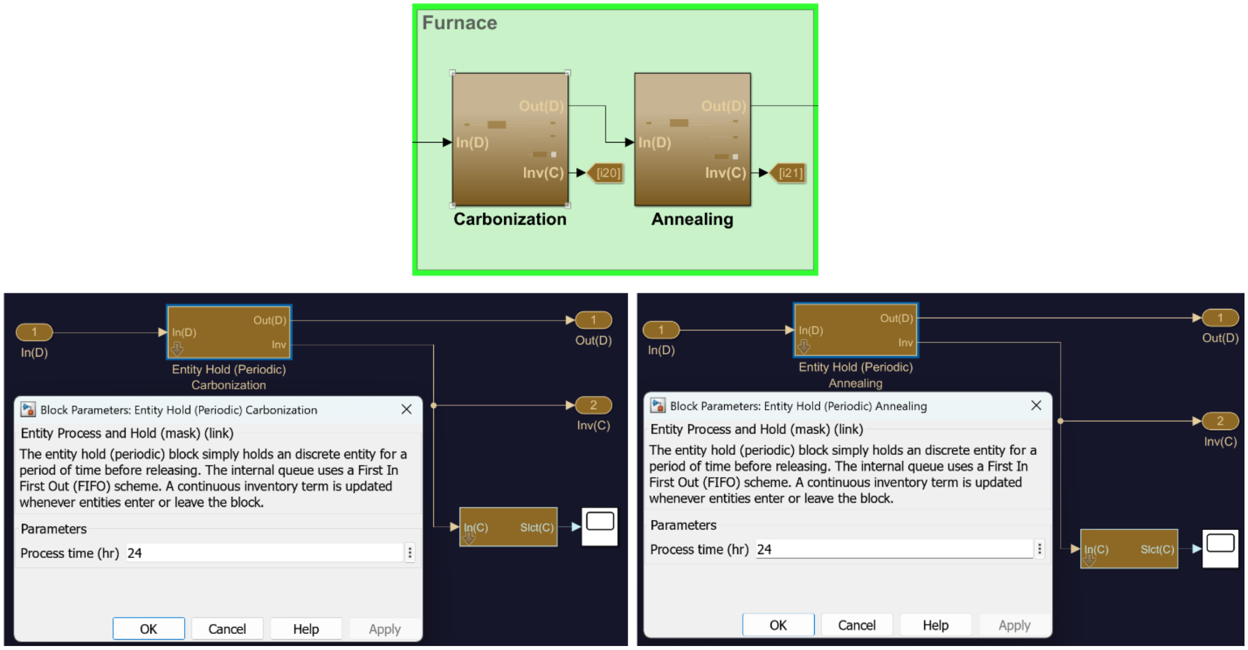

Figure A-17. TRISO fuel carbonization and annealing sections of the TRISO fuel fabrication F3M model.

Table A-27. TRISO fuel carbonization and annealing process times in the TRISO fuel fabrication F3M model.

Parameter	Value	Units
Carbonization process time	24	hr
Annealing process time	24	hr

A.2.3.3 Final fuel form manufacturing

As noted in Section 2.1.4.3, the TRISO fuel fabrication F3M model includes a final fuel form manufacturing step, which could include processes such as loading TRISO compacts into graphite prismatic blocks or fuel inspections. Figure A-18 shows the final fuel form manufacturing section of the F3M model, while Table A-28 shows the process time.

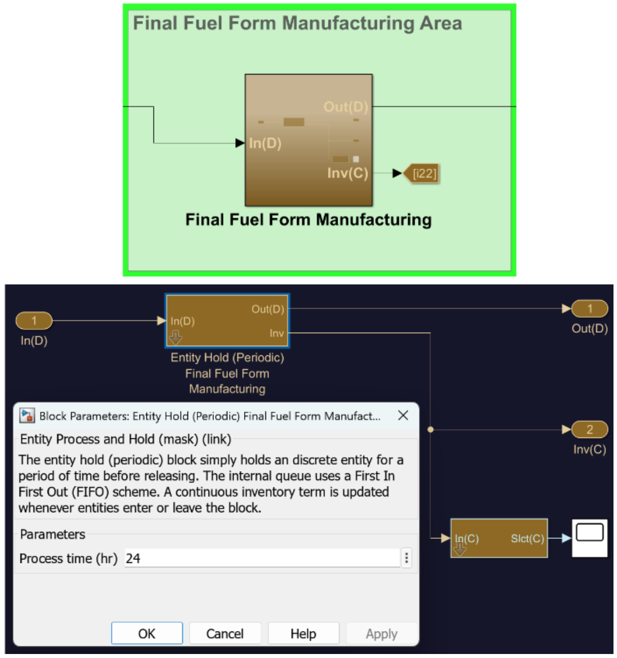

Figure A-18. TRISO final fuel form manufacturing section of the TRISO fuel fabrication F3M model.

Table A-28. TRISO final fuel form manufacturing process time in the TRISO fuel fabrication F3M model.

Parameter	Value	Units
Final fuel form manufacturing process time	24	hr

A.3. Material Balance Area 3: Final TRISO Fuel Form Storage

As mentioned in Section 2.1.6, MBA 3 consists only of the final TRISO fuel form storage and drum packaging area. The model framework in FY25 focused on the generation of inputs, inventories, and outputs for MBA 2; therefore, MBA 3 simply serves as a landing area for the TRISO final fuel form outputs. Figure A-19 shows the TRISO final fuel form interim storage and drum packaging area; Table A-29 shows the parameters associated with interim storage and drum packaging.

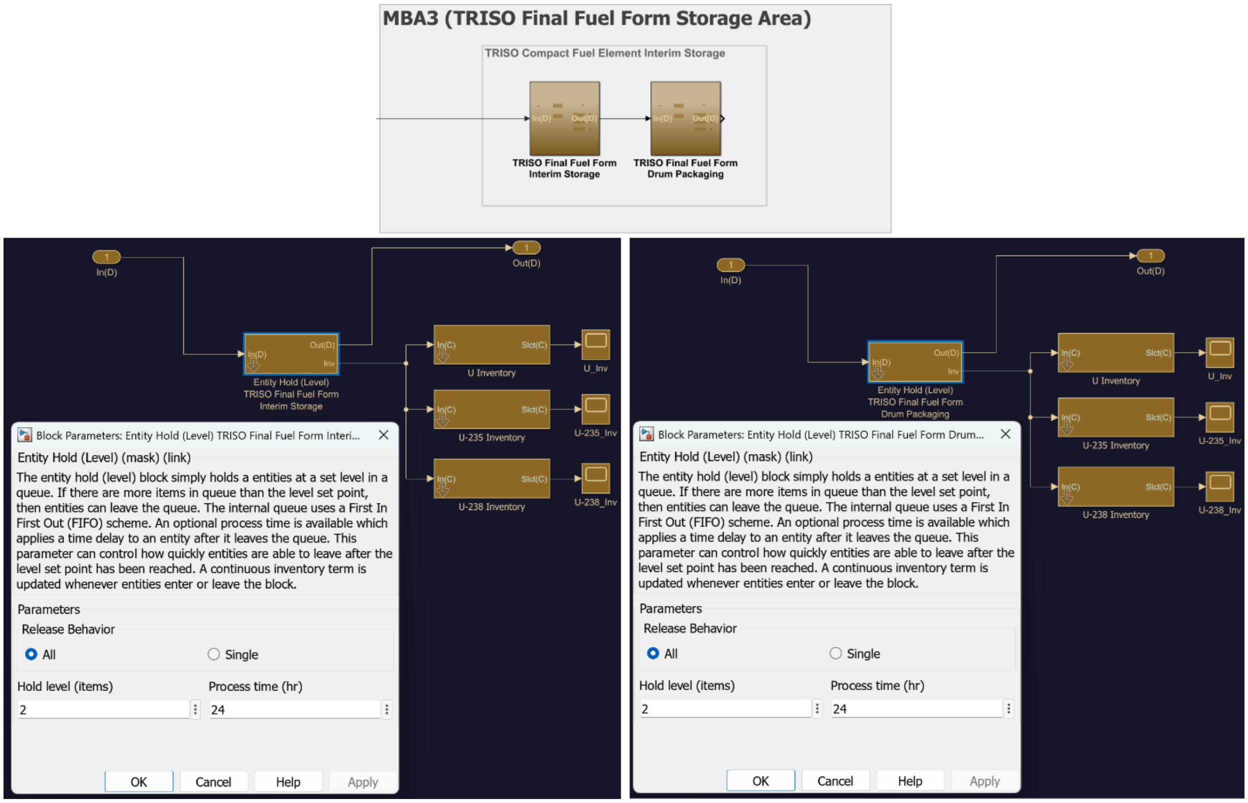

Figure A-19. TRISO final fuel form interim storage and drum packaging section of the TRISO fuel fabrication F3M model.

Table A-29. TRISO final fuel form interim storage and drum packaging parameters in the TRISO fuel fabrication F3M model.

Parameter	Value	Units
Final fuel form interim storage hold level	15	items
Final fuel form interim storage process time	24	hr
Final fuel form drum packaging hold level	2	items
Final fuel form drum packaging process time	24	hr

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