

# Nuclear Fuel Cycle and Supply Chain (NFCSC) Technical Monthly August FY-22

Changing the World's Energy Future

August 2022



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August 2022

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## 1. ADVANCED FUELS CAMPAIGN (AFC)

# 1.1 Industry FOA

#### 1.1.1 GEATFFOA

**[LANL]** GE Bi-lateral Activities, FT-22LA02010302 Fabrication of <sup>235</sup>U enriched UO<sub>2</sub> composite pellets for BR2 irradiation test have been fabricated and are undergoing characterization. Preliminary density measurements show that densities are > 94% TD. Thermophysical properties measurements on deplete analogue samples have shown a 25% improvement of the thermal conductivity relative to UO<sub>2</sub> pellets. Pellets will be packaged and shipped following characterization activities.

### 1.2 ATF Lab Activities

#### 1.2.1 ATF FABRICATION PROPERTIES

**[LANL]** Accelerated irradiation and qualification of ceramic nuclear fuels, FT-22LA02020104 FAST tests, sample enrichment/geometries, and insertion timeline have been defined and will be included in an upcoming status report.

#### 1.2.2 ATF CORE MATERIALS

**[ORNL]** Fabrication and Characterization of Coated Cladding, FT22OR02020204 The AFC Level 3 Milestone M3FT-22OR020202043 – "Summarizing Effect of Coating Thickness and Condition on Behavior of Zr Cladding" due on August 5th was successfully completed. The ORNL report (ORNL/SPR-2022/2539) provides a comprehensive summary of the impact of coating thickness on the mechanical properties of coated Zr.

Two batches of High-Power Impulse Magnetron Sputtered (HIPIMS) Cr-coated Zry-4 cladding tubes have been produced and successful tested for reproducibility of coating application. 7-micron thick coatings were compared to 30-micron thick cold sprayed Cr-coatings to assess the impact of coating thickness on performance. The coating processes generated different microstructural features which may impact coating performance. Scanning and transmission electron microscopy was used to assess differences in grain sizes and orientations and the crucial interface between the two coating techniques. The interface was investigated on an atomic level for a potential Laves phase formation, but none was found in as-coated condition. The cold sprayed and HiPIMS coating interface differs dramatically. The cold spraying process deforms and partially recrystallizes the Zry-4 cladding tubes at the surface, whereas the HiPIMS coatings do not appear to impact the cladding substrate. The cold spray process reduces the Zry-4 grain size in the interface region resulting in deformation and heat induced recrystallization. This deformation caused by the cold spray results in a wavy interface between the Zry-cladding (black) and the Cr grain (colorful), see Figure 1. Conversely, these observations were not present in the HiPIMS coated material.

Simulated loss-of-coolant accident (LOCA) testing was performed following microstructure characterization to assess differences in mechanical performance. LOCA burst testing results indicate a neglectable impact of the thickness at lower pressures, however, the HiPIMS materials consistently ruptured at higher temperatures than the cold spray at higher pressures shown in Figure 2. Posttest analysis indicated the grain sizes and coating density impacted the mechanical properties and LOCA performance. However, the impact of a coating thickness on corrosion properties is still unknown and will be determined in a systematic study in FY23.

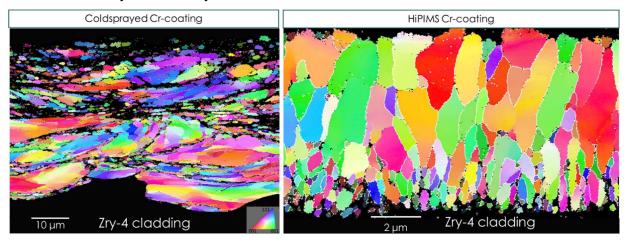


Figure 1. Inverse pole figure maps of backscattered electron diffraction patterns from cold sprayed (right) and HiPIMS (left) Cr-coatings. the bottom in black represents the Zry-4 cladding. Be aware of different scale bars between the micrographs.

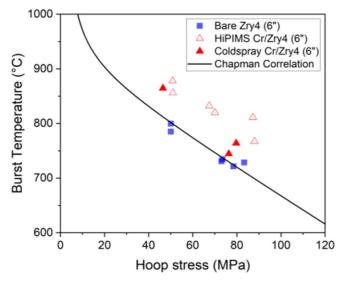


Figure 2. Burst temperature plotted against hoop stress for ORNL sourced HiPMS and coldspray cladding tubes in comparison to bare Zry4.

### 1.2.3 ATF IRRADIATION TESTING

**[INL]** Integral Irradiation Testing, FT-22IN02020301 ATF-2C hardware and pin fabrication activities continued to support experiment insertion in the Advanced Test Reactor 2A Loop during Cycle 171A. ATF-2C will consist of four tiers. Tier 1 (bottom tier) and Tier 2 will include Framatome fueled pins, Tier

3 will include General Atomics empty SiC tubes, and the top tier (Tier 4/5/6) will be Mitsubishi developed alloy clad UO2 pins, two equipped with temperature sensors, two with pressure sensors, and two non-instrumented. M2FT-22IN020203015, "ATF-2C test train top tier assembled and ready for insertion was completed August 25, 2022.

#### 1.2.4 ATF SAFETY TESTING

[INL] HERA, FT-22IN02020402 The safety analysis package for the HERA experiment campaign was completed and allows the experiment capsules to be irradiated. The first transient on the calibration capsule was completed, and the second capsule build was completed and is ready to be transferred to the reactor. The paperwork for the instrumentation on the first two prehydrided capsules was approved. The pellets for the prehydrided tests were ground and the end caps for the rodlets were welded and radiographed.

**[INL]** Integral Transient Testing, FT-22IN02020403 The project team has been dissecting and rewriting FORTRAN code utilizing a more modern mathematics tool that is more flexible for a graphite core. The new tool should more appropriately predict the epithermal and fast neutron fluxes. In addition, foils are being prepared to support characterization work of the BUSTER pipe inside of the TREAT core.

#### 1.2.5 ATF PIE

**[INL]** ATF Post Irradiation Examination, FT-22IN02020501 The in-cell qualification of the VEM ministage has been completed to meet the upcoming level 3 milestone due at the end of August.

The analyses of the ring hoop tension test used to support the qualification of ATF cladding has been completed and the draft of the manuscript is being edited.

#### 1.3 Advanced Reactor Fuels

#### 1.3.1 AR IRRADIATION TESTING

**[INL]** AF Irradiation Testing, FT-22IN02030301 Pre-conceptual design work is on-going for the Boosted Energy Advanced Spectrum Test (BEAST). Design work includes various neutronic and thermal-hydraulic studies of various test rig concepts utilizing flux-trap positions in the ATR.

FAST-1 capsules are in the ATR canal storage awaiting ATR insertion and the start of 171A-1 cycle irradiations. Transfer to the vessel will be performed either during the nuclear testing (NT) cycle or the 171A-1 outage, which is significantly delayed due to issues with the nuclear testing (NT) cycle at the ATR. ATR 171A-1 cycle-specific analyses are on-going.

PIE work in HFEF remains on-going. JFCS AFC-IRT-1 C3 & C4 specimens are in storage with exams complete. PIE continuation of AFC-3F, AFC-4C & EBR-II X-486 specimen is on-going. Gamma scanning is now complete for both 4C and 3F. AFC-3F and AFC-4C disassembly is concluded. One rodlet of AFC-3F remained stuck inside the capsule tube and it will need to be processed through the mill in HFEF. AFC-4C rodlets have now completed profilometry and neutron radiography. Sectioning of EBR-II X-486 is now complete with metallography and sampling work still on-going. FAST-1 non-destructive exams were completed previously. FAST-1 destructive exams are awaiting GASR modifications, which are in-process with an expected completion at the end-of-August. The LIFT advanced characterization work is on-going. This characterization work is expected to conclude by the end of the fiscal year.

[INL] Accelerated Fuel Development and Qualification Methodology Development, FT-22IN02030302 Investigation of metallic fuel scalability for the purpose of reactor-agnostic metallic fuel qualification — Completed BISON model of a FAST experiment to emulate an EBR-2 irradiation.

Setting the stage for accelerated fuel development and qualification with an engineering-driven real-world case study – The trade study has now been completed and that the manuscript is now under preparation.

Thermodynamically described separate effects testing to support accelerated fuel development and qualification – XRD has been completed for all samples at ambient temperature. In situ heating has been completed for U-10Zr and U-30Zr. U-6Zr is awaiting repair of vacuum pump. Data analysis has begun. SEM/FIB has started on select U-Zr samples. Four FIB lamella have been collected for TEM analysis. TEM will follow in the coming weeks. During SEM/FIB time, BSE, SE, and select EDS was performed for characterization.

**Demonstration of process similitude on metallic fuel experiments** – No accomplishments. Work is slow to start due to not enough resources available for the work currently. Working on getting additional resources to support the work.

**[LANL]** Accelerated Compositional Effects Testing, FT-22LA02030304, Accelerated Compositional Effects Testing Ion irradiations under two different modalities completed.

Characterization is currently underway, although delayed due to equipment maintenance for the past month.

Initial report will be furnished by end of FY, if schedule holds (i.e., no more equipment maintenance).

#### 1.3.2 AR SAFETY TESTING

[INL] ARES – Joint work with JAEA to study off-normal behavior of fast reactor fuels, FT-22IN02030401 Completion INL milestone M3FT-22IN0203040113 titled "Complete a summary report of the pre-transient characterization of the AFC metallic pins".

The THOR-C-2 has been irradiated. Instrumentation, hodoscope, and radiograph data look good. Preliminary data indicates that THOR-C-3 accomplished the purpose of the experiment to melt the fuel.

Capsule assembly and fuel fabrication of THOR-C-3 is complete.

The fuel capsule assembly of THOR-C-3 is nearing completion.

Pre-characterization of the JAEA MOX pins at HFEF is ongoing and preliminary results have been shared with JAEA.

The THOR-M final design review has been closed and recorded.

The Remote Handling HFEF THOR team is nearing completion of the fabrication and qualification of the HFEF handling fixtures. (T. Smuin)

**[INL]** Sodium loop commissioning experiments – prelim design complete, FT-22IN02030402 Work Package is no longer active.

#### 1.3.3 AR PERFORMANCE ASSESSMENT

**[INL]** AFC Advanced Reactor Fuels Performance Assessment, FT-22IN02030501 Milestone report draft under development regarding image analysis for constituent redistribution identification from irradiated metallic fuel radiographs.

Full fuel performance analyses for FFTF MFF-2 and MMF-6 experiments have been completed. Code and model updates are forthcoming to improve calculation efficiency and improve fuel swelling predictions. Discussion started about type of report and desired data to be reported to summarize the results effectively for AFC users.

## 1.4 Silicon-Carbide Cladding

# 1.4.1 SIC CLADDING (FOA)

[INL] INL Post Irradiation Examinations (SiC), FT-2W2IN02050102 Completed preliminary testing for SiC cladding using thermal property microscope, and we engaged with the GA team to synergize experiments and characterization to support their new initiative on accelerated fuel qualification. We are also completed the draft of the SiC PIE capability gap assessment report, which will be issued by 09/30.

# 1.5 Capability Development

#### 1.5.1 ATR LOOP INSTALLATION

[INL] Design and Install I-loop), FT-22IN02060101 Through August 2022 with approximately \$7.342 million of project to date completed work scope including the design, fabrication, and installation of the THCP, the project is ahead schedule and below budget with a project to date SPI of 1.04 and a CPI of 1.14. Based on the availability of staff resources, engineering design continued to be accelerated. The acceleration with resulting productivity increase continued to increase the positive cost variance in labor. Cost savings will be utilized to support future procurement of materials, equipment, and services where cost and schedule are uncertain with a significant risk in the supply chain. The Accomplishments in August 2022 include the following.

- 1. The Preliminary Project Execution Plan (PLN-6297) was completed and approved.
- 2. The F&OR (FOR-482) was approved and issued.
- 3. The review of the Transfer Shield Plate and Shield Cylinder Upgrade TFR (TFR-2566) was completed, and the DCR review of the I Loop Tube (TFR-2569) was initiated.
- 4. Drawings were submitted to DCR review and to planning in support of the ripout of existing 1A cubicle and basement equipment.
- 5. Heater options of the I loop system pressurizer concept were identified to reduce cost and maintenance time, and the conceptual model of the loop transmitter cabinet was completed.
- 6. Initiated preparation of the submittal of the Zr-2.5NB prototype procurement through the new INL eMarketplace (ARIBA) tool and continued to explore Canadian import/export control issue resolution.
- 7. Initiated design and development of a detailed schedule of a stainless-steel I Loop Tube prototype to accomplish initial mechanical interface testing.



Figure 3. Image: 3D Image of I-Loop Tubes Installed in ATR's I-13 and I-14 Medium-I Positions

#### 1.5.2 TREAT LOCA TESTING INFRASTRUCTURE

**[INL]** TWIST (RIA/LOCA), FT-22IN02060201 The TWIST final design and analyses were completed, and a final design review kick-off meeting and presentation held. Additional analysis was done for the OPTI-TWIST assembly, and progress was made on the machine shop work package for the OPTI-TWIST modifications.

#### 1.5.3 REFABRICATION AND INSTRUMENTATION CAPABILITY

**[INL]** TREAT Reinstrumentation Capability (non-capital), FT-22IN02060301 Completed development of the draft fiscal year end milestone progress report for re-instrumentation and submitted for review.

Engineers from the Institute for Energy, formerly known as the Halden Reactor Project, began development of a pre-conceptual design document focused on a vertically oriented cryogenic drilling system.

For more information on Fuels contact Steven Hayes (208) 526-7255.

### 2. MATERIAL RECOVERY AND WASTE FORMS DEVELOPMENT

#### 2.1 EBR-II Acceleration

[INL] Completed receipt of the 11<sup>th</sup> & 12<sup>th</sup> of 12 planned FY-22 EBR-II driver fuel shipments at FCF.

- Receipt of a 13<sup>th</sup> shipment is under consideration for September.

Completed moisture inspection on fuel bottles from the 10<sup>th</sup> and 11<sup>th</sup> FY22 fuel shipment to FCF from INTEC.

Continued FY22 treatment operations.

- Completed element preparation and electrorefining of the 6<sup>th</sup> and 7<sup>th</sup> of 8 planned treatment batches.

Commenced HALEU regulus production at the cathode processor.

- Five of 7 planned drip casting runs were completed in August, producing nearly 215 kg of HALEU in regulus form.

Completed 3 additional casting furnace runs in FCF to produce HALEU parent ingots, bringing total to 8 of a targeted 9.

- The resulting HALEU parent ingots are being cast into regulus shape during August & September of FY22.

#### 2.2 Zircex

[INL] A manuscript entitled, "Radiolytic Evaluation of Select Sulfur Chlorides (S<sub>2</sub>Cl<sub>2</sub> and SOCl<sub>2</sub>) for Advanced Low Temperature Chlorination of Zirconium-Based Used Nuclear Fuel Cladding," was written and submitted to Radiation Physics and Chemistry (Impact Factor = 2.858, 2022). The research discussed within covers our findings from over the last year: (i) both sulfur chloride compounds exhibited significant radiation resistance, with respect to changes in the Raman signatures of the parent compounds and the ingrowth of Raman-active degradation products; (ii) molecular chlorine (Cl<sub>2</sub>) was directly identified as the predominant degradation product from S<sub>2</sub>Cl<sub>2</sub> radiolysis, and was completely consumed at higher absorbed doses (> 9.27 MGy); (iii) similarly, the main degradation product from SOCl<sub>2</sub> radiolysis was also Cl<sub>2</sub>, although in this medium it continued to grow in with dose over the entire dose range; (iv) an "S=O" containing degradation product(s) was also identified as a compliment to Cl<sub>2</sub> in SOCl<sub>2</sub>; and (v) the perceived radiation resistance of these sulfur chloride compounds makes them suitable for inclusion in a used nuclear fuel chemical decladding process, especially as radiolytically formed Cl<sub>2</sub> can be used to reform the parent compounds, thereby increasing the longevity of the solvents used.

**[ORNL]** Alternative chlorination is being investigated as a way of separating and reclaiming zirconium from spent nuclear fuel. A manuscript has been drafted on the chemistry of zirconium recycling, "A Novel Protocol to Recycle Zirconium from Zircaloy Cladding from Spent Nuclear Fuel Rods." The primary authors on this publication are Breanna Vestal and Dr. Craig Barnes from the University of Tennessee Knoxville, funded by DOE-NE through an NEUP. Participation of DOE-NE-43 through Oak Ridge National Laboratory from the beginning of the NEUP to the completion is acknowledged in the manuscript. This work is the basis for further investigation of this process for Zircex now continuing at ORNL.

#### [INL] HALEU Design & Support

- Began fabrication on HC Loader
- Work continued on the HC fluidized bed analysis

#### [INL] Zircex Polishing

- Removal of enclosure is complete

[PNNL] PNNL has received the Raman spectrometer from INL and is beginning the collection of optical training sets.

[PNNL] PNNL has drafted a journal article that documents the corrosion behavior of the in-can canister material (Inconel 601 alloy) in borosilicate glass melts at 1100°C. INCONEL 601 crucibles showed corrosion was mainly along the grain boundary, at a corrosion at a rate of 22 mm/y, see Figure 1. Figure 2 shows the electrochemical corrosion measurements of Inconel 601 coupons began at a corrosion rate of 60 mm/y [low resistance polarization (Rp)] but the rate slowed with time to approximately 10 mm/y after 150 h of testing as the Rp increased over time. The Inconel 601 alloy forms eskolaite (Cr<sub>2</sub>O<sub>3</sub>) skin that likely reduces further corrosion (see Figure 1). Additionally, inside the corroded grain boundaries it forms Al<sub>2</sub>O<sub>3</sub> that may also hinder corrosion. This verifies the likely success of the in-can melting technology materials of construction choice of Inconel 601 and demonstrates the baseline glass formulation for use with in-can melting.

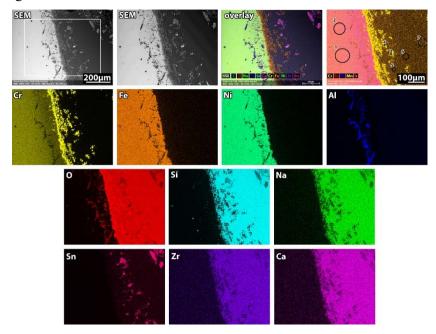


Figure 4. BSE, overlay, and elemental map images of the of Inconel 601 crucible to glass (A-9.17) interface midway down the side wall of the crucible after heat treatment at 1100°C for 300h. Images show elemental distributions in the Inconel 601 alloy and glass. The overlay image shows the major phases: Inconel 601(green), Cr<sub>2</sub>O<sub>3</sub>(orange), SnO<sub>2</sub>(pink) and glass (dark grey), less apparent is the Al-O rich regions in the alloy.

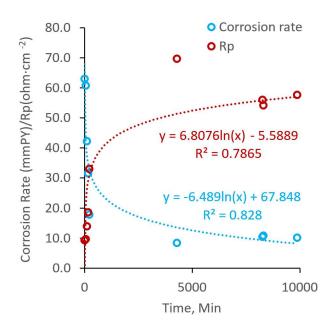


Figure 5. Corrosion rate and resistance polarization (R<sub>p</sub>) of Inconel 601 versus time in A-9.17Sn glass melt at 1100°C, with natural logarithm fits to each.

[ANL] As noted previously, the current loading module uses simplified mathematical species representations similar to that used in the previous Excel version. However, the existing aqueous and organic speciation equations for individual species, and the associated equilibrium data, employed in the current MATLAB code can be used to solve for TBP loading which should provide more accurate values at high loading. To that end, the existing D-value equation modules for the uranium, americium and nitric acid were modified to derive the aqueous and organic phase equations needed to fully develop this approach. The loading module uses these formulations to construct mass balance equations, which are then used to build the Jacobian needed to iteratively solve for the individual component loading in the solvent. This new implementation of the loading module is still being refined, and the calculated results obtained compared with those obtained with the previous version to assure that the implementation is accurate. The initial results show somewhat higher D-values for uranyl and americium but the code will be verified and the output validated using experimental data. (C. Pereira)

#### 2.3 Off-Gas & Waste Forms

[ANL] Initial tests with iron phosphate materials produced at PNNL and Clemson by using different processing methods to assess effectiveness of processes and intrinsic durabilities of the materials have been completed and analyses are in progress. An informal workshop with UK researchers was hosted on Aug. 24 to discuss possible collaborations related to waste forms. Argonne recommended possible collaborations addressing test methodologies, data analyses, and waste form selection that are being considered. Iodide waste form materials with different I<sub>2</sub> loadings provided by ORNL and PNNL were characterized and prepared for use in immersion and electrochemical tests.

**[PNNL]** PNNL completed milestone M4FT-22PN030104042 "Ship iodine-loaded Ag-aerogel waste form to ANL for chemical durability testing". Iodine loaded silver-functionalized silica aerogel (Ag<sup>0</sup>-aerogel) was immobilized with spark plasma sintering or with low-temperature encapsulation process, which was developed to address a need for an easily employed, reliable, and on-site production of durable waste forms. An invention disclosure record was submitted for this process and for composition variation of

low-temperature durable matrices. Fully densified product was obtained for "Durable Matrix/iodine-loaded Ag<sup>0</sup>-aerogel" fraction 75/25 vol% with iodine loading ~16 mass%. Produced waste forms were shipped to ANL for chemical durability testing.

# 2.4 Single Cycle Aqueous Separations

[ORNL] Previously, we reported a stronger binding affinity of 2-amino-5-nitrobenzimidazole (ANBI) with pertechnetate (TcO<sub>4</sub><sup>-</sup>) over nitrate (NO<sub>3</sub><sup>-</sup>), whereas all other investigated ligands exhibited the opposite trend. To better understand this result, we examined the structure of the two anion-ANBI complexes and discovered that nitrate was deprotonating the N atom in the ring during optimization in gas phase, whereas pertechnetate was not deprotonating the ligand. This proved to be an artifact of the optimization procedure and deprotonation was not observed when optimization was performed in the presence of an implicit solvent. This re-examination now suggests that ANBI behaves similarly to all previously examined ligands.

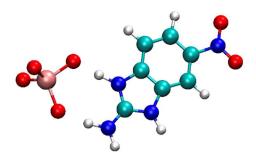


Figure 6. 2-amino-5-nitrobenzimidazole interacting with pertechnetate. (O = red, C = cyan, N = dark blue, H = white, Tc = pink).

[PNNL] The report Single-Cycle Flowsheet Testing Plan was completed to fulfill milestone number M4FT-22PN030101042. This report provides recommendations for advancing U recycling flowsheets to the point of demonstration with dissolved fuel. Several options for single-cycle U recycling flowsheets can be considered, each of these options being influenced to some degree by the outcomes of the ongoing R&D activities that are briefly described in this report. A strategy for developing the flowsheet options to the point of demonstration is provided. The report first summarizes the ongoing process chemistry investigations that are relevant to flowsheet development. Potential U recycling flowsheet options are then described, along with how the ongoing R&D activities influence flowsheet development. The report concludes with a generalized approach for planning flowsheet demonstrations. The report will be submitted in early September to complete the milestone.

# 2.5 Pyrochemical & Molten Salt Processes

[ANL] A report summarizing successful sequential actinide and lanthanide drawdown tests that demonstrate the range of separation and operational control was submitted. Tests using more complex multi-component salts are in progress. Drawdown products were prepared for use in waste form development.

[INL] A contract for fabrication of the co-deposition assembly will be awarded upon receipt of bids from external vendors. Bids are due on September 14th. A report documenting the design of the co-deposition assembly has been drafted as well. A report documenting the progress of the filtered salt sampling apparatus has been drafted and will be completed on time to satisfy the milestone delivery date. A report documenting the findings of the INL MFC Analytical Laboratory to develop and validate methods for

uranium oxychloride, oxide, and metal samples was generated and a memo documenting its completion was uploaded to PICs. For FY22, this work primarily focused on validation of ethyl acetate-bromine dissolution procedures for determination of oxide and metal fractions of a uranium sample. This report is currently undergoing export control review and when completed will be available upon request from William Phillips at william.phillips@inl.gov.

**[INL]** An inventory of replacement remote distillation system components was compiled to complete a level 4 milestone in August.

## 2.6 Aqueous Separation Science & Novel Processes

[ANL] Data from the literature and collected at PNNL for Pu<sup>4+</sup> extraction with DEHiBA (N,N-di(2-ethylhexyl)isobutyramide) have been reviewed and pre-processed for inclusion in a Pu<sup>4+</sup>-DEHiBA extraction model. A preliminary model fit of the data is in preparation. The DEHiBA extraction models will utilize the refinements being made to the AMUSE loading module to calculate the concentration of free extractant available for forming complexes.

[INL] Aqueous Separation Science & Novel Processes, FT-22IN03040202, A report "Extraction of technetium by DEH*i*BA in liquid-liquid systems containing uranium and zirconium," has been completed, fulfilling the milestone M4FT-22IN030402021. The acquired data summarized in the report supported PNNL's characterization of solvent extraction properties of single-cycle solvent formulation based on DEH*i*BA monoamide extractant. Distribution of technetium was evaluated for a reference solvent. Technetium extraction from a range of aqueous nitric acid and uranyl nitrate concentrations was monitored, where all aqueous mixtures contained 300 mg L<sup>-1</sup> Tc-99 and 0.03 mol L<sup>-1</sup> Zr. In general, a 2-fold increase in the efficiency of transfer of technetium into non-aqueous environment containing DEHiBA was observed, relative to traditional PUREX solvent based on tributylphosphate.

**[ORNL]** NO<sub>2</sub>-voloxidation is being investigated as a way for preparing spent nuclear fuel for direct dissolution without using copious quantities of HNO<sub>3</sub>. Although NO<sub>2</sub>-voloxidation has been studied in the past at Oak Ridge National Laboratory, the tests were preliminary and have not provided sufficient information for quantitative analysis or scaling. Hence, parametric tests are now being carried out on NO<sub>2</sub>-voloxidation in a bench-scale apparatus. Initial testing has been done using sintered UO<sub>2</sub> pellets to determine the optimal conditions for producing a uranyl nitrate product. The process includes multiple steps, forming U<sub>3</sub>O<sub>8</sub>, and UO<sub>3</sub> before the nitrate. Previous reports have suggested that the addition of a hydration step, reacting the UO<sub>3</sub> with steam, is optional, serving to only increase reaction rate. However, we have determined that it is necessary for the nitration to occur. The results of the parametric tests are being documented in a report that will be completed at the end of September.

[SRNL] The hazard analysis for studying the dissolution kinetics of selected lanthanide oxides in a tributyl phosphate (TBP)/dodecane solvent was approved. The initial experiments will evaluate the dissolution of neodymium oxide (Nd<sub>2</sub>O<sub>3</sub>) in 30 vol % TBP at ambient temperature. The TBP solvent will be pre-equilibrated with 10 M nitric acid to provide sufficient extracted acid in the TBP to solubilize the Nd<sub>2</sub>O<sub>3</sub> as neodymium nitrate (Nd(NO<sub>3</sub>)<sub>3</sub>). A dip probe in the TBP dissolution vessel connected by fiber optic cable to a UV-vis spectrometer will be used for in situ measurement of the dissolved Nd(NO<sub>3</sub>)<sub>3</sub> concentration. X-ray absorption spectroscopy will be use in tandem with the UV-vis spectrometer to assist in quantifying the amount of completely dissolved oxide at trace levels.

# 2.7 Innovative Salt Systems

[ANL] The performance of novel double-junction reference electrodes made using different combinations of porous separators and ionically-conductive membranes is being evaluated. A status report summarizing

the approach and initial results was issued (ANL/CFCT 22/27) and analyses of other systems are in progress.

A chloride gas electrode was designed for use in direct chlorination experiments. Initial experiments have been planned for chlorination of uranium dendrites and hazard assessments have been initiated. The design is suitable for chlorinating approximately 1 kg of uranium metal.

**[INL]** analysis continued on salt crystallization experiments completed on LiCl-KCl with cesium and sodium to study the ability of removal of these species. The experiments showed strong promise for separating cesium and follow-on experiments have been set up. Later experiments will explore rare earth removal from the same system. A chloride volatility apparatus has been prototyped and has undergone initial testing in a non-rad laboratory glovebox with molten salt. Preparations are under way for initial experiments utilizing HCl gas.

**[ORNL]** During the reported period, we studied the solubility of La2O3 in LiCl-KCl-MgCl2 mixtures with 5wt%, 20wt%, and 50wt% of MgCl2 at 750 °C. We also measured the solubility of Nd2O3 in the same salt compositions in the 450-750 °C temperature range using the isothermal saturation method.

The purchase order for the zone refining system was placed and made it through the ORNL internal purchasing system. I spoke with a representative from the company, and they have received the order and are starting the final design for the system.

We have successfully installed and tested the LAMMPS-DeePMD interface for running MD inference using the trained DeePMD neural network potentials on the Summit supercomputer after much effort. We are now prepared to perform both training and inference (i.e., run simulations with the DNN potential) on Summit. We have also submitted an application for a Director's Discretion allocation on Summit in order to benchmark our training and simulation pipeline, in order to prepare for an ALCC leadership allocation competition. We have performed simulations with VASP using two different functionals on the AlCl3 100% system, for 5 different volumes, for 30 ps each. We are now performing these simulations on various ratios of KCl and AlCl3. These simulations will be used for training a general neural network potential for AlCl3/KCl systems. We have also created a new workflow software to perform many parallel VASP simulations in preparation for enhanced sampling simulations on the molten salts in order to explore the potential energy surface. The workflow has been tested on 75 nodes (450 GPUs) of Summit, with each worker running several consecutive jobs successfully. As opposed to bulk, solid systems, a number of different species are formed in molten salts, and these evolve over rather long timescales compared to the time required to run these AIMD simulations. Therefore, improved sampling of these transitions with enhanced sampling methods will provide the data needed to train a general force field capable of simulating chemical reactions and rare events.

**[PNNL]** The team has tested three significant modifications of probe design, indicating a clear path forward for controlling sensitivity for customizable application to very dark chemical targets (e.g. U(III)) or weak chemical targets (e.g. low concentration Nd).

For more information on Material Recovery and Waste Forms Development contact Ken Marsden (208) 533-7864.

#### 3. MPACT CAMPAIGN

# 3.1 Campaign Management

#### 3.1.1 NTD & MANAGEMENT SUPPORT

**[LANL]** MPACT Federal Program Manager, NTD, and Deputy NTD attended the NE-4 FY23 Planning Meeting, where NTD presented on MPACT's proposed FY23 planning packages, work packages, and budget allocations. NTD and Deputy NTD attended the NEUP webinar. MPACT Federal Program Manager, CAM, Deputy NTD, and NTD completed FY23 planning package activities and began drafting FY23 work packages.

#### 3.1.2 CAMPAIGN MANAGEMENT

**[BNL]** Supported the National Technical Director with preparations and support for NE-4 FY23 Planning Meeting, preparation and support during NEUP Webinar, participated in weekly MPACT meetings, supported FY23 work package development.

## 3.2 Front-End Domestic Safeguards

#### 3.2.1 ENRICHMENT PLANT

**[BNL]** BNL and other MPACT laboratories are negotiating the NDA language with Centrus. At this point, there are only a few points to be resolved and BNL is in routine contact with Centrus and the other national laborites to resolve all outstanding issues. BNL expects to sign the NDA is September.

**[ORNL]** The MCNP analysis for the online enrichment monitor (OLEM) to support potential use for HALEU has been completed.

#### 3.2.2 FUEL FABRICATION - HOLDUP

[ORNL] Testing began in ORNL safeguards laboratory.

#### 3.2.3 FUEL FABRICATION - MODELING

**[SNL]** The fuel fabrication modeling report was completed in early August and describes the capabilities of the safeguards model. This LEU model will form the basis for future work on varying fuel fabrication designs.

#### 3.2.4 NMAC TRAINING

**[LANL]** Timeline, design documents, and training modules are nearing completion. Minimal further course development will be needed in first quarter of FY23. Ideally, we will bring in strategic expertise to attend a pilot course.

**[BNL]** Modifications to the NMAC program design to customize the training to the needs of the target audience and clarify the learning objectives and training approaches.

[SNL] Met with the team recently to go over feedback on the first NMAC training module and to continue planning the remainder of the training.

### 3.2.5 FUEL FABRICATION - STANDARDS

**[ORNL]** Bi-weekly discussions with Westinghouse continued as ORNL provided technical support to their lead engineer.

#### 3.2.6 AR FUEL FABRICATION NMAC STUDY

**[LANL]** New LANL fuel fabrication SME began engaging with the multi-lab team to develop the report summarizing U.S. advanced reactor fuel fabrication methods and identifying potential gaps in the current process.

# 3.3 Back-End Domestic Safeguards

#### 3.3.1 ELECTROCHEMICAL & AQUEOUS SPIKE-BASED REPROCESSING NMAC

**[INL]** Data analysis of the FY22 Na-22 spiked salt samples has been completed. The results show that the radioactive tracer dilution technique and gamma spectroscopy is feasible for total mass measurement of molten salt systems, though the improvement of uncertainty of gamma spectroscopy is desired. The uncertainty improvement will be investigated in FY23. The draft journal publication (M2), "Development, feasibility and uncertainty of radioactive tracer dilution coupled with gamma spectroscopy for molten salt mass determination" has been completed and is under INL review.

# 3.3.2 ELECTROCHEMICAL & AQUEOUS REPROCESSING ACOUSTIC INTERROGATION

**[LANL]** Work focused on preparing for the Level 2 Milestone measurements in September. Acoustic sensor systems underwent final build tests and calibrations for the Level 2 testing.

#### 3.3.3 MOLTEN SALT PM/NMA

[ANL] Monitoring of the HFEF electrorefiner is continuing. Additional scenarios have been monitored including clean-up operations. Final analyses of the FY22 activities are being performed for the end-of-year milestone report.

[INL] Finished electrorefiner run 1 and are preparing to operate batch 2 in the electrofiner.

#### 3.3.4 Reprocessing Sampler

[ANL] The molten salt sampler has been transferred into the glovebox and is being prepared for installation into one of Argonne's electrorefiners. Wiring for the heater zones has been completed and also transferred into the box. Operations of the sampler are planned for September.

#### 3.3.5 Reprocessing Modeling

[SNL] The MC&A portion of the Zircex model has been updated. Currently working on final report.

#### 3.3.6 MICROCALORIMETRY

**[LANL]** Training and first measurements at the Idaho National Laboratory Materials and Fuels Complex Analytical Laboratory were successfully completed in August. Work began with installing the updated multiplexing electronics and third detector assembly. Analytical Lab staff were trained in operation of the system including instrument operation for routine measurements and common scenarios such as power outages, and data processing. First measurements were collected on a dissolved electrorefiner salt sample which showed the value of the instrument in resolving low-energy peaks that are not accessible with the AL's germanium detectors. The instrument is now operational by AL staff with a subset of detector channels providing good performance. The remaining detector channels were observed to be affected by heating and poor resolution; solving these problems to recover system detection efficiency will be the focus in the short term.

**[INL]** The microcal instrument is operating and samples from the MPACT Na-22 Spiking project at INL have been measured.

#### 3.3.7 PSMC MEASUREMENTS

**[INL]** The repaired and tested PSMC junction box was shipped to INL. The install and testing will occur the last week of September.

For more information on MPACT contact Mike Browne at (505) 665-5056.

# 4. SYSTEMS ANALYSIS AND INTEGRATION (SA&I) CAMPAIGN

4.1 CAMPAIGN MANAGEMENT

[INL] Attended the NE-4 planning meeting Aug. 3-4 and presented campaign planning information. In a separated session, presented information on the PNAS journal article claiming significantly higher waste production from advanced reactors, identifying where claims had validity and where support was missing or claims were based on worst-in-class performance.

[INL, ANL] Developed FY-23 planning package content, including drafting scope of activities and tasks, identifying lead and contributing labs, determining funding splits, and identifying milestones.

## 4.2 NUCLEAR ENERGY SYSTEM PERFORMANCE (NESP)

# 4.2.1 Scenario Analysis and Technology Roadmap Studies of Fuel Cycle Facilities for Demonstration Reactors

**[ORNL]** Generated a draft report documenting the work on Xe-100 type pebble bed reactor modeling in SCALE. The model confirmed that high burnup can be achieved in pebble bed reactors, as noted by X-Energy in their papers and presentations. In addition, the SCALE calculations showed that the pebbles adjacent to the reflector experience a slightly higher thermal-to-fast flux ratio. As a result, these pebbles near the reflector experience much higher burnups than the pebbles near the center of the core where the thermal-to-fast flux ratio is lower. Therefore, the pebble pathway through the core during the 6 passes does affect the burnup.

# 4.2.2 Investigate Benefits and Challenges of Converting Retiring Coal Plants into Nuclear Plants

[INL] Staff worked with C2N team members from ANL and ORNL to finalize the milestone report for external release. INL staff worked closely with communications staff form DOE-NE, supporting their effort to prepare a press release that announced the C2N report and summarized findings. INL staff met with staff from GAIN for foundational work on a C2N analysis for a coal community GAIN works with.

**[ORNL]** Provided support and made efforts to make the case study site anonymous in the C2N report, and also incorporated DOE-NE review feedback into the C2N report.

# 4.2.3 Nuclear Roles for Electricity Market Reliability in Deep Decarbonization Scenarios

[ANL, BNL] Submitted a milestone report, "Nuclear Roles for Electricity Market Reliability in Deep Decarbonization Scenarios" by Nicolas Staff et al. This report is the deliverable in the fulfillment of the Level 3 milestone, M3FT-22AN120102013 under the work package of "FT-22AN12010201 Nuclear Energy System Performance (NESP) - ANL."

The Systems Analysis and Integration campaign has analyzed the benefits of nuclear power in deeply decarbonized electric grids through detailed electricity market modeling of Texas and the continental United States with the A-LEAF code. The scenarios with a high fraction of nuclear capacity had fewer unserved electricity hours during a severe weather event due to higher availability and dispatchability and lower outage rates, while a high fraction of VRE had larger unserved electricity

hours. This study observed that when nuclear power plants were available with unconstrained capacity and moderate cost, they enabled lower system costs than renewable-and-storage-only scenarios in most cases due to higher required solar and wind capacity increasing the generation capital expenses and fixed O&M cost.

# 4.2.4 DEVELOP FUEL CYCLE DATA PACKAGES AND UPDATE/MAINTAIN OF NUCLEAR FUEL CYCLE OPTIONS CATALOG

[ANL] Developed the system datasheet of a once-through fuel cycle option with HALEU sodium-free U-Zr metallic fuel in an SFR. The reactor performance parameters were obtained from a PRISM/Mod B core that was modified to simulate TerraPower's Natrium. The nuclear fuel technology datasheet of a sodium-free metallic fuel was also developed. Both system datasheet and technology datafile are under review internally and externally based on the FCDP development procedure.

[SNL] Continued to work toward moving the catalog to the O365 SharePoint cloud and to work with the Sandia personnel responsible for setting up the cloud to ensure that they understand the catalog's requirements. We were able to gain access to a test environment on the cloud to test the database and the database reporting functions. Those tests are currently in progress and have helped to identify areas where the transition from the old system to the new system will not be seamless. The transition can still occur, but it will require additional programming work.

#### 4.2.5 QUICK TURN-AROUND STUDIES

[ANL] Waste characteristics of SMRs (NuScale, Natrium, and Xe-100) were evaluated using the normalized metrics of discharge fuel mass, SNF volume, decay heat, radiotoxicity, GTCC volume, and LLW volume to unit electricity generation (GWe-year). Compared to a large-size LWR, non-LWR advanced SMRs (Natrium and Xe-100) generate smaller amounts of discharge fuel mass, decay heat, and radiotoxicity because those metrics are inversely proportional to the burnup and thermal efficiency. However, SMRs generate more or similar disposal waste volume (GTCC + SNF) depending on reactor types. A further wide-range activation analysis with SMR vendor's design information is needed to evaluate LLW volume accurately. The waste characteristics and observations were presented at the NE-4 planning meeting (Aug 3-4, 2022).

#### 4.2.6 SUPPORT DOE NE IN INTERNATIONAL ENGAGEMENTS

**[INL]** Continued discussions on the content of the economics chapter of the report for the NEA Task Force on Demonstration of the Fuel Cycle Closure including Partitioning and Transmutation for Industrial Readiness by 2050.

#### 4.2.7 FUEL CYCLE ANALYSIS TO SUPPORT TECHNOLOGY CAMPAIGNS

[INL, ANL, SNL] Conducted discussions with multiple campaigns in NE-4, 5, and 8 to identify and develop planning information for collaborations in FY-23.

# 4.3 ECONOMIC AND MARKET ANALYSIS FOR NUCLEAR ENERGY SYSTEMS (EMANES)

#### 4.3.1 GLOBAL AND REGIONAL NUCLEAR ENERGY USE FOR THE 21ST CENTURY

[PNNL] The report "Scenarios of Nuclear Energy Use in the United States for the 21st Century" by Sonny Kim was submitted in fulfillment of Level 2 milestone, M2FT-22PN120103051 under work package FT-22PN12010305 Economic and Market Analysis for Nuclear Energy Systems (EMANES) – PNNL. This report investigates the potential range and timing of future nuclear energy contributions to the US energy system. The interactions of improved nuclear competitiveness through nuclear reactor capital cost reductions and alternative climate mitigation policies are explored to assess the potential expansion of nuclear power throughout the 21st century. Multiple long-term scenarios of the US energy system are generated using the PNNL GCAM model for clarifying the role of nuclear capital cost reductions, the role of carbon penalties and emission constraints, and their combined impact on the deployment of nuclear power and on carbon emissions in the US.

#### 4.3.2 Costing and Techno-economic Assessment Automation

[ANL, INL] Submitted the report entitled "Costing and Techno-economic Assessment Automation" by E. Hoffman et al. This report is the deliverable in the fulfillment of the Level 4 milestone, M4FT-22AN120103013 under the work package of "FT-22AN12010301 Economic and Market Analysis for Nuclear Energy Systems (EMANES) - ANL."

The core functionality of computer software to automate the Algorithm for the Capital Cost Estimation of Reactor Technologies (ACCERT) methodology was developed in FY 2022. Significant progress on ACCERT software development was accomplished. The basic concept and approach for the ACCERT software have been completed by implementing a relational database and coded algorithms. The current version of the ACCERT software has been demonstrated that could generate the cost report for the PWR-BE direct capital costs. The envisioned evolution of the ACCERT software for estimating the whole Levelized cost by adding the functionality of separate categorization and treatment of different types of cost (e.g., capital and O&M) are also addressed in the report.

#### 4.3.3 Cost Basis Report Improvement/Update

[INL, ANL, SNL] The report "FY-22 Annual Report on Improvements and Updates to the Advanced Fuel Cycle Cost Basis Report" by Jason Hansen et al, was submitted in completion of milestone M3FT-22IN120103032, This report describes the improvements and updates conducted this fiscal year. These include a new cost module for HALEU enrichment, the first ever CBR case study (developed to show how to use the report) on back-end fuel costs and updates of 3 associated back-end modules, and an approach for adding new cost data on MSRs and microreactors.

[INL, SNL] INL staff completed the final draft of the annual update report on improvements and updates to the Cost Basis Report. Supported with content from SNL, ORNL and ANL, the update report documents the new cost data on HALEU cost impacts to enrichment, among other updates.

#### 4.3.4 Market-Driven Competitiveness of Nuclear Power Plants

[ANL] Continued assessing the impact of natural gas availability and cost on the market price of electricity and nuclear revenues. Various scenarios were analyzed, and the results will be discussed in an upcoming report.

#### 4.3.5 Reprocessing System Trade Studies

**[ANL]** Completed the hiring process of Dr. Nick Soelberg as Argonne Associate. Held a kick-off meeting with the MRWFD campaign (July 27) for a basic understanding of the voloxidation off-gas treatment technology.

**[INL]** INL staff worked provided feedback to industry partner MUNRO for input on final report on factory fabrication. Further, continued working on the M3 milestone due at the end of the FY.

For more information on Systems Analysis and Integration contact Brent Dixon (208) 526-4928.

#### 5. AFCI-HQ PROGRAM SUPPORT

Site: University Research Alliance at West Texas A&M University in Canyon TX, and the following universities: Purdue University, Massachusetts Institute of Technology, Georgia Institute of Technology, Pennsylvania State University, North Carolina State University, University of Tennessee at Knoxville, Washington State University, Colorado School of Mines, University of California at Santa Barbara, University of South Carolina, University of Central Florida, Clemson University, Virginia Commonwealth University, Air Force Institute of Technology, University of Michigan, University of Texas at Austin, Coastal Carolina University, Missouri University of Science and Technology, University of Illinois at Urbana-Champaign, and other universities.

#### Universities engaged in Nuclear Technology research via URA programs since 2001:

Boise State University

University of California at Berkeley
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Clemson University University of California at Davis

Colorado School of Mines

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Technology
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Pennsylvania State University
University of Utah
Purdue University
University of Virginia
University of Wisconsin

Rensselaer Polytechnic Institute University of Wisconsin Rutgers University Vanderbilt University

Texas A&M University

Virginia Commonwealth University

University of Arkansas Washington State University

# 5.1 Innovations in Nuclear Technology R&D Awards

### 5.1.1 UNIVERSITY PROGRAMS

#### 5.1.1.1 Summary Report

University Research Alliance provided information to the First Place Innovations Awards winners and worked with the award winners and the American Nuclear Society on the Innovations in Nuclear Technology R&D Awards special session, to be held during the ANS Winter Meeting November 13-17.

University Research Alliance prepared materials to order award trophies for the 2022 Innovations Awards winners.

University Research Alliance continued to update the Innovations Awards announcement distribution list in anticipation of the 2023 Innovations Awards.

For more information on the University Research Alliance contact Cathy Dixon (806) 651-3401.