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Roadmap for IES Modeling and Simulation Activities

September 2022

Changing the World's Energy Future

Aaron S Epiney, Paul W Talbot, Rami M Saeed, Daniel S Wendt, Daniel Garrett, Mohammad Gamal M Mostafa Abdo, Ramon Ken Yoshiura, Jun Soo Yoo, Daniel Mark Mikkelson, Jason K Hansen, Elizabeth Kirkpatrick Worsham, Shannon M Bragg-Sitton

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IES

Integrated Energy Systems

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ABSTRACT

Since inception of the DOE-NE Integrated Energy Systems (IES) program, several program and modeling visions and roadmaps have been published. In 2017, the last modeling and simulation capability development plan was published. In 2020, a comprehensive roadmap for the DOE-NE Integrated Energy Systems program was published. The current report is meant to update the 2017 modeling and simulation capability roadmap and complement the IES overall program roadmap published in 2020.

The role of modeling and simulation within IES is to support the demonstration of new coupled integrated technologies along every step of the technology maturation from the strategic analysis of preferred system architecture to preliminary design, to laboratory testing, up to full commercial testing and integration. To achieve this role, modeling and simulation must be able to assess the technical performance and the economic viability of potential IES. Also, modeling and simulation must provide support for experimental evaluations (i.e., support component design and real-time operations of experimental demonstration systems). Finally, modeling and simulation can help scale-up experimental systems to the final commercial systems.

This report details the current state of the modeling and simulation efforts within IES for the above-mentioned areas, provides a gap analysis, and proposes next steps for a time horizon over the next 4 to 5 years.

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CONTENTS

FIGURES

TABLES

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ACRONYMS

AHP	Analytical Hierarchy Process
ANL	Argonne National Laboratory
A-NPPs	Advanced NPPs
ARMA	Auto-Regressive Moving Average
CDF	Cumulative Distribution Functions
CG	Command Governor
CHP	Chemical Heat Pumps
DETAIL	Dynamic Energy Technology and Integration Laboratory
DISPATCHES	Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems
DMDc	Dynamic Mode Decomposition with Control
DME	Dimethyl Ether
DRAFT	Dynamic Reliability Analysis Framework and Toolbox
DSS	Dynamical System Scaling
ERCOT	Electric Reliability Council of Texas
ES	Electrical Storage
FARM	Feasible Actuator Range Modifier
FASTR	Facility to Alleviate Salt Technology Risks
FMI/FMU	Functional Mockup Interface / Unit
FOM	figure of merit
FORCE	Framework for Optimization of ResourCes and Economics ecosystem
FT	Fischer-Tropsch
GHGs	Greenhouse gases
GMI	Grid Modernization Initiative
H2TS	Hierarchical Two-Tiered Scaling
HERON	Holistic Energy Resource Optimization Network
HTGR	High-Temperature Gas Reactor
HTE	High Temperature Electrolysis
HTSE	High Temperature Steam Electrolysis

HX	Heat Exchangers
IEA	International Energy Agency
IES	Integrated Energy Systems
LDRD	Laboratory Directed Research and Development
LMP	Local Marginal Prices
LSTM	Long-Short Term Memory
LWRS	Light Water Reactor Sustainability program
MAGNET	Microreactor Agile Non-nuclear Experimental Test Bed
MFSP	Minimum Fuel Selling Price
MIMO	Multiple-Input-Multiple-Output
MOAS	Maximum Output Admissible Set
MPC	Model-based Predictive Control
MSR	Molten Salt Reactor
MTO/MOGD	Methanol-to-olefins to gasoline and distillate
NEUP	Nuclear Energy University Program
NGNP	Next Generation Nuclear Plant
NPP	Nuclear Power Plant
NPV	Net Present Value
N-R HES	Nuclear-Renewable Hybrid Energy Systems
O&M	Operation and Maintenance
ORCA	Optimization of Real-time Capacity Allocation
ORNL	Oak Ridge National Laboratory
PCM	Physics-guided Coverage Mapping
PID	proportional–integral–derivative
PNNL	Pacific Northwest National Laboratory
PVGS	Palo Verde Generation Station
QFD	Quality Function Deployment
RAVEN	Risk Analysis Virtual Environment
ReEDS	Regional Energy Deployment System

RFE	Recursive Feature Elimination
RG	Reference Governor
ROM	Reduced-order Model
RTO	Real-time Time Optimization
RWD	Random Window Decomposition
SAF	Sustainable Aviation Fuel
SFR	sodium-cooled fast reactor
SMRSIMO	Small Modular Reactors Single-Input-Multiple-Output
SOECSMR	Solid-oxide Electrolysis Cell Small Modular Reactors
SQL	Structured Query Language
NoSQL	Not Only SQL
TESTEDS	Thermal Energy Storage Thermal Energy Distribution System
TSA	Time-Series Analysis
TTSSTES	Thermocline Thermal Storage System Thermal Energy Storage
V&VUQTTSS	Validation and Verification Uncertainty Quantification Thermocline Thermal Storage System
VARV&VUQ	Value at Risk Validation and Verification Uncertainty Quantification
VREVARV&V	Variable Renewable Energy Value at Risk Validation and Verification
VREVAR	Variable Renewable Energy Value at Risk
VRE	Variable Renewable Energy

Roadmap for IES Modeling and Simulation Activates

1 INTRODUCTION

Since the inception of the DOE-NE Integrated Energy Systems (IES) program, several program and modeling visions and roadmaps have been published.

- In 2017, the last modeling and simulation capability development plan was published [1]. This document assessed the needed modeling and simulation capability for Nuclear-Renewable Hybrid Energy Systems (N-R HES). The report focused on the following key capabilities:
    - The creation of the system boundary conditions (e.g., the capability to create stochastic input data, such as demand profiles, renewable supply histories, and price profiles)
    - The creation of a numerical representation of the physical model of an N-R HES system
    - The derivation of the cash flow from the actual performance of the physical system to perform the economic assessment
    - The optimization of N-R HES configuration (capacities) and dispatch.
- In 2020, a comprehensive roadmap for the DOE-NE IES program was published [2]. This document focused more broadly on the current state of nuclear technologies, high-priority heat users, and interface technologies for IES. The report also analyzed gaps and barriers in implementing new IES technologies. The needed modeling and simulation support was only briefly discussed in a short chapter.

This current report is meant to update the 2017 modeling and simulation capability roadmap and complement the IES overall program roadmap published in 2020. This report will first summarize and update the main priorities from the 2020 overall IES technology roadmap, then assess the status of the IES modeling and simulation framework and finally assess gaps and make suggestions for future modeling and simulation activities and capability developments.

1.1 Integrated Energy Systems Program Mission

Many cities, states, utilities, and public commissions are setting energy standards that aim to reduce carbon emissions. To realize a clean and resilient energy future, new methods of energy production, distribution, and use will be required. Renewable energy technologies are currently being deployed in significant numbers around the world in response to the desire to reduce emissions, coupled with decreasing costs for these technologies. However, despite this growth, data reported in the International Energy Agency's *Future of Nuclear* report that was released in May 2019 indicate that the fraction of clean energy contributions to electricity generation has not changed over the last 20 years. This unexpected trend results from the increasing penetration of variable sources driving nuclear energy out of the market in some regions and resulting in the shutdown of some large-scale, non-emitting plants when non-emitting renewable resources are added to the grid. The advent of historically low-cost renewable generation sources, alongside low cost and high availability of natural gas, has driven down the price of electricity, decreasing the minimum baseload generation required to meet load at certain times of the day or year. These factors serve to diminish the role of traditionally baseload nuclear generation. While many nuclear plants have responded to increasing volatility in net demand by operating flexibly, reducing power output to losses when market prices are very low or negative. While this practice preserves the contribution of nuclear energy to grid stability, it diminishes the economic value of operating nuclear plants in these regions. Nuclear energy is a proven low-emission option that can provide consistent, dispatchable power to meet electricity demands while also providing high-quality heat that can meet energy demands beyond the electricity sector.

The mission statement of the IES program is [2]:

"Maximize energy utilization, generator profitability, and grid reliability and resilience through novel systems integration and process design, using nuclear energy resources across all energy sectors in coordination with other generators on the grid."

The vision to achieve this is [2]:

"A robust and economically viable fleet of light-water and advanced nuclear reactors available to support [U.S.] clean baseload electricity needs, while also operating flexibly to support a broad range of non-electric products and grid services."

The IES program defines proposed integrated nuclear-renewable energy systems and identifies key technology gaps to realizing the deployment of commercial-scale systems for the production of a variety of electric and non-electric products. IES under consideration could incorporate multiple energy generation resources and energy use paths, with a focus on low-emission technologies such as nuclear and renewable generators. Together these technologies provide affordable, reliable, and resilient energy while simultaneously reducing environmental emission of CO_2 and greenhouse gases (GHGs).

Integrated Energy Systems are cooperatively controlled systems that dynamically apportion thermal and/or electrical energy to provide responsive generation to the power grid. They are comprised of multiple subsystems, which may or may not be geographically co-located, including a nuclear heat generation source, a turbine that converts thermal energy to electricity, at least one renewable energy source, and one or more industrial processes that utilize heat and/or power from the energy sources to produce a commodity-scale product. IES design and optimization would consider both technical performance and economic viability within various deployment markets. Various subsystem designs, integration options, and deployment scenarios are considered in evaluating gaps to commercial-scale deployment of IES.

Nuclear energy can provide consistent, dispatchable power to meet electricity demands while also providing high-quality heat that can meet energy demands beyond the electricity sector—all without emission of CO_2 or other GHGs. To fully realize these benefits, it is necessary to better characterize the potential role or roles for nuclear energy amid the growing field of variable renewable generation technologies. As described, IES that leverage nuclear energy generation systems can effectively touch all major manufacturing industries, including fuels, chemicals, metals, and the paper product industries, as well as smaller industries associated with food production, biofuels plants, minerals concentration, and water purification.

Coupled energy generation systems (e.g., novel reactor technologies) and advanced industrial applications may not be commercially deployed at present, but the necessary steps toward technology maturation are being addressed through various federal R&D investments and private industry investment. These advances in the technical readiness of independent components and subsystems will provide much needed performance data to validate and improve modeling, simulation, and optimization of integrated systems that may employ these technologies. Key technology gaps specifically associated with IES applications include advancement of the readiness level of components for heat transport and heat exchange across diverse systems, thermal energy storage, heat augmentation, electricity management, and control systems developed specifically for IES that can safely and securely manage the multi-application nature of IES.

1.2 Modeling and Simulation Support

The goal of the IES program to successfully fulfil its vision is [2]:

"The IES program develops tools and technologies that will lead to demonstration of multiple integrated energy systems that have a clear path toward commercialization. Timelines follow the associated reactor concepts and designs (current fleet now, advanced 5-15 years)."

Integration of energy generation, storage, and use technologies present different technical, economic, and regulatory challenges for electrical and thermal integration approaches. R&D is needed to demonstrate coordinated delivery of the two energy streams in IES, particularly given that electrical power and thermal energy are delivered through systems with significantly different time scales and inertia. Much of the necessary R&D for maturation of integrated systems focuses on integration technologies, the development and validation of the models used to design and optimize IES for specific regional applications, and establishing regulatory approaches that are suited to the unique design and implementation options for IES.

Technology maturation will be accomplished via multiple R&D pathways for system and process modeling and simulation; component development, testing, and demonstration at increasing scale; development and demonstration of system monitoring and control approaches and tools; and an integrated system demonstration. Notional timelines for development of IES for light-water reactors (LWRs), light-water, small-modular reactors, and advanced reactors have been proposed, noting that the necessary research may be completed by various federal and private industry research programs. One priority area of research that will be addressed by the DOE-NE CTD-IES program, in coordination and partnership with industry when appropriate, are advanced reactors. The proposed deployment timeline for advanced reactor technology is shown in Figure 1.

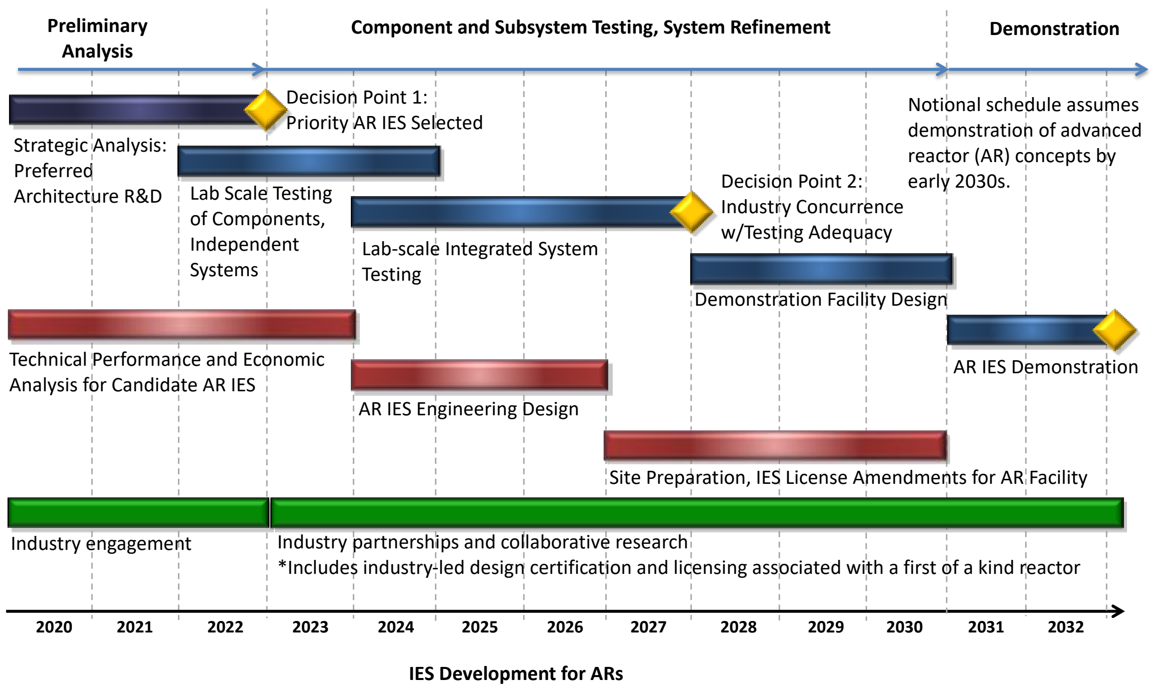


Figure 1. Notional IES deployment timeline for advanced reactors. Start date of 2020 reflects large-scale advanced reactors. Microreactors may be demonstrated on a shorter timeline and could include IES applications [2].

The role of modeling and simulation within IES is to support the demonstration of new coupled integrated technologies along every step of the technology maturation from the strategic analysis of preferred system architecture to preliminary design, to laboratory testing, up to full commercial testing and integration.

The key areas modeling and simulation must address are:

- ***System Simulation***
  - ***Technical Performance***. Develop and exercise an ecosystem for modeling, analysis, and optimization of IES that can accommodate various reactor types, renewable technologies, and energy users. This includes steady-state analysis of IES to assess technology compatibility (temperature range, mass flows, etc.) as well as time-dependent physics calculations to evaluate dynamic interactions of different components of IES. This includes overall system ramping capabilities, operational transients, such as coupled system startup and shutdown, as well as deterministic safety analysis (e.g., what is the overall system response if one component suddenly becomes unavailable).
  - ***Economic Analysis***. Establish a reference capability to validate current practices in valuing nuclear energy in the energy market (electric and non-electric). This includes steady-state economics to assess the market potential of an IES but also detailed time-dependent techno-economics to assess the stochastically optimal assets mix (energy and industrial heat/electricity users) as well as energy/commodity arbitrage scenarios in different multi-market scenarios.
- ***Simulation Support for Experimental Evaluation***. The experimental campaign within IES seeks to establish and operate a fully functional and diverse non-nuclear facility for model validation and initial technology demonstration as well as nuclear IES demonstrations in partnerships with related DOE programs and industry. The modeling and simulation support for the experimental demonstrations includes:
  - ***Component Design***. Establish a framework to help select technologies and optimize the design of individual components of an IES. While industry already has or is working on reference designs for heat/electricity producers such as advanced nuclear plants as well as heat/electricity users, such as hydrogen or chemical production plants, the IES program is focusing on intermediate technologies to couple individual components of IES. In other words, the IES program tries to fill the gap between individual component design and the integrated final system. These connecting intermediate technologies include advanced heat exchangers as well as heat augmentation systems.
  - ***Real-time Optimization***. Develop a reference capability to control IES in real time. This includes the development of digital twins (DT) for individual components of IES including acquisition of real-time data from sensors, faster than real-time physics simulations of the system, and feedback of control actions to be taken by the system. The DT framework answers the question of how to operate a system in real time to reach optimal economics (how to react to markets and dispatch assets in real time) as well as how to operate the IES from a technical and control perspective, (e.g., how to develop and implement governing control systems for the couped IES system).
  - ***Scaling***. Develop a computational framework to scale individual components from laboratory testing to final industrial application. This includes process scale-up and error propagation in scaled models as well as the capability to adjust input/output relations between different components of an IES during experiments. For example, if two experiments at different laboratories are integrated virtually, the real-time input/output scaling can adjust signals coming from one experiment before they are transmitted to the other facility.

1.3 Analysis Approach and Tools

The IES program has established a computational framework that leverages advanced modeling and simulation tools developed through the support of multiple DOE-NE programs while incorporating specialized tools necessary for the economic optimization of integrated systems. The overall framework is called the Framework for Optimization of ResourCes and Economics (FORCE) ecosystem. This framework is applied to conduct analysis of the technical and economic viability of a range of possible IES configurations and, at the end, to optimize those configurations within a specific U.S. region. The analysis tools and approach are briefly summarized in Figure 2 and described in more detail in later sections.

The first step in evaluating a candidate IES is to determine the technical feasibility of the system. High-fidelity tools, where "high" fidelity is relative to the level of complexity of the systems modeled, are used to determine the steady-state performance of the IES configuration to derive efficiency of the thermochemical processes and necessary scaling factors to assess plant costs. This step is performed primarily using commercial tools, such as ASPEN HYSYS.

Following this step, the dynamic aspects of the systems are assessed by creating a dynamic model of the plant in the Modelica language. These models are used to determine controllability of the system, characteristic ramp rates, and overall operability in transient situations. A common control system needs to be designed and tested to ensure that coordination among the different components/subsystems is achieved, and no component exceeds its technical limits.

Modelica models are usually relatively slow to run for the number of years necessary to perform financial evaluation of the investment (usually 30+ years); therefore, surrogate models are usually adopted in the next step of the process. The original Modelica models are run when the time horizon is short, and the analysis is more focused on capturing the ability of the IES to respond to the dynamic nature of the market. When this type of simulation is performed, the accelerated aging of components needs to be captured to provide negative financial feedback that derives from the corresponding increase in maintenance costs, shorter asset lifetimes, and asset replacement. Accelerated aging models to capture this aspect of performance represent a gap in IES development and deployment; however, such models are currently under development by the CTD-IES program.

At the next step, the Holistic Energy Resource Optimization Network (HERON) tool is used to optimize the dispatch of different IES resources to the grid or the co-product markets (inner loop in right side of Figure 2) and to optimize the individual component sizes within the IES (outer loop in right side of Figure 2). HERON implements a stochastic optimization approach to manage the stochastic nature of the market itself. During the dispatch optimization in which the response of the IES as a whole is optimized, advanced control strategies are necessary. Control systems appropriate to IES represent a current technology gap that is being studied by CTD-IES.

Among optimization dispatch analysis tools, HERON is the first to adopt a fully stochastic approach; such an approach is now being followed by other commercial tools. Therefore, some challenges are expected. Most of the future needed work in this respect is focused on reduction of the necessary number of samples to ensure a reliable convergence of the stochastic optimization under probabilistic constraints.

At present, there are still gaps in regard to the various analysis tools necessary to support refinement of IES design that must precede commercial deployment. First, long-term portfolios are not yet defined in the analysis framework; hence, there are no capacity expansion features in HERON. For IES analyses completed thus far, long-term portfolio projections have been conducted using the Regional Energy Deployment System (ReEDS) tool developed by the National Renewable Energy Laboratory, and if needed, market clearing has been assessed using PLEXOS. While these tools can provide input to the HERON analysis, they don't have the capabilities for a complete techno economic analysis like HERON. IES is seeking collaboration with other partners to couple existing capacity expansion and market interaction tools that will further enhance HERON capabilities.

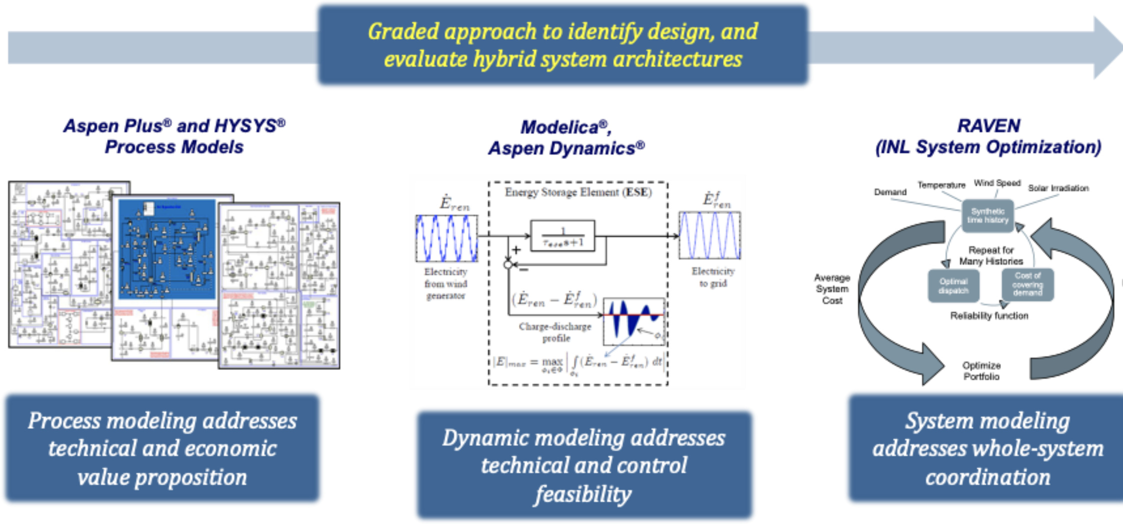


Figure 2. Summary of analysis approach being applied for IES configurations. For a higher resolution and explanation of the picture on the right, see Figure 13.

Once technical and economic viabilities have been demonstrated, the IES moves to experimental demonstration. This usually starts with laboratory scale testing and then moves to larger demonstrations as the technology matures. Two additional FORCE modeling capabilities are currently developed that will support the experimental technology demonstrations: real-time optimization (RTO) and scaling.

RTO uses similar simulation functionalities as the techno-economics tool HERON (dispatch optimization, economic evaluations) but exercises them in real time while the assets are working and not a priory during the system design phase. The planned avenue for RTO within FORCE is through DT. The DT collects the sensor data and sends it to the RTO tool within FORCE. The RTO tool then optimizes the system actions (under constraints from a covering control system) with respect to best economics (or other figures of merit, such as energy efficiency or GHG emissions) and sends control actions back to the different assets through the DT framework.

IES will incorporate modern scaling techniques such as dynamic system scaling (DSS) [3], physical coverage mapping [4], and non-linear representativity. These methodologies can simulate how laboratory scale demonstrations will scale up to the full production scale. In particular, the methodologies allow users to assess the simulation uncertainty of full-scale models knowing the uncertainty in the simulation model relative to the experiment (through measured experimental data). Also, these methodologies can be used to inform model validation by assessing the validation domain of the different models. A corollary of this capability is that the methodologies inform the experimental campaigns to maximize the validation domain for models. The DSS, Physics-guided Coverage Mapping (PCM), and representativity methodologies are currently being implemented in Risk Analysis Virtual Environment (RAVEN) and are part of the FORCE tool suite.

As mentioned, modeling and simulation has a support function in the IES program. Software capabilities are driven by "use cases." Industry and government priorities drive the selection of use cases and associated technical and economic questions. Figure 3 shows how use cases inform the simulation framework and experimental campaigns. Experiments also inform software requirements. The outcomes of the simulation software then back-inform the use cases and experimental campaigns as described earlier in this section. **This report will (1) summarize an already investigated use case and propose future ones; (2) summarize how modeling and simulation can inform experimental campaigns and technology demonstrations, and (3) summarize the current capabilities of the FORCE tools and propose new capabilities needed to support future use cases and experimental demonstrations.**

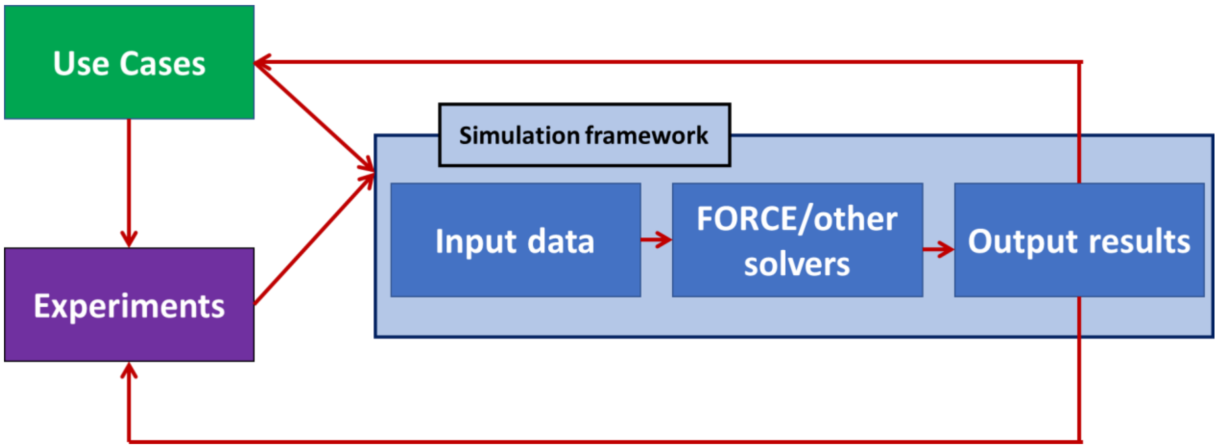


Figure 3. IES modeling and simulation framework.

2 APPLICATION CASES

This section gives details about the IES application cases that have been and are currently under investigation by the IES program. Application cases are split in three categories: (1) techno-economic demonstrations, (2) modeling and simulation support for experimental demonstrations, and (3) technology interconnections.

2.1 Techno-economics Demonstrations

Techno-economic demonstrations involve various aspects for a proposed IES. The final goal of the techno-economic demonstrations is to assess the economic viability of the proposed system in a defined market setting considering the physical dynamic constraints of the system (i.e., obtain a comparison of cost and revenues). The costs include construction costs for new systems as well as fixed and variable operating costs. The main gap to address in this category is the cost functions for advanced reactor technologies. On the revenue side, the market structure in which the IES is operating needs to be understood in detail. While the program developed a general understanding of how the different regulated and deregulated markets in the U.S. work, there are still gaps, in particular understanding the impact of regional policies and incentives on the profitability of nuclear systems.

To be able to include the physical dynamic constraints of the system in the analysis, industrial requirements (thermal and electrical) for heat/electricity generators (advanced reactors), thermal storage, and potential industrial applications must be known. This includes limitations on internal process variables, such as temperatures, pressures, mass flows, etc., as well as dynamic limits of the system to ramp up and down.

Possible industrial processes that could benefit from electrical and thermal coupling with nuclear energy have been identified (see Figure 4). The plan of the IES program is to develop and expand a chart/table that ranks/classifies the possible use cases by different criteria. Among them are technology maturity, cost, general market economics/potential, energy efficiency, social justice, environmental justice (GHG reduction potential), resilience, reliability, and safety (transient, cyber, and licensing).

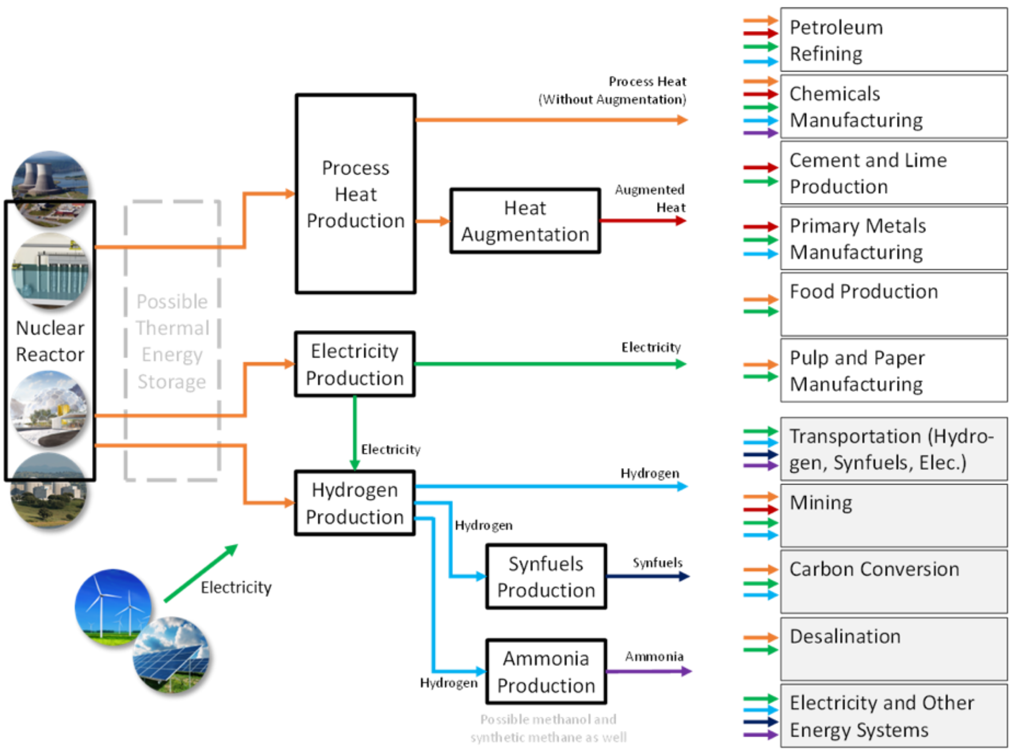


Figure 4. Potential industrial applications for direct electrical and thermal coupling with nuclear power [5].

In addition, the program plans to develop a methodology to analyze use cases from a techno-economic perspective, such that different technologies can be compared on a technical basis beyond expert opinion and adding additional aspects related to acceptance (i.e., move from techno-economics to techno-socio-licensing-economic).

The following subchapters summarize the status of the techno-economics for use cases currently under investigation by the program and identifies future work potential.

2.1.1 Water Desalination

Considering nuclear-driven desalination, IES analyzed a case study in partnership with Arizona Public Service (APS) in 2018 and 2019 [6, 7]. As a U.S.-specific example, the municipalities west of Phoenix, Arizona are presently challenged to sustain growth due to the limited water resources. As groundwater and surface water resources are stressed, these municipalities are now focusing on other, lower quality brackish groundwater resources that are available and sustainable in large supply. Use of this resource is dependent on cost-effective desalination and management of the process concentrate or reject stream. There are limited options for the management of the treatment process concentrate from a large-scale municipal water treatment facility. Deep well injection is improbable in the shallow Phoenix sub-basin, and the injection process presently lacks the required authority in Arizona. Surface evaporation ponds are very expensive and require significant surface area for the large-scale municipal projects. These options are high cost and thus provide an incentive to consider other more cost effective, innovative options. The Palo Verde Generating Station is located nearby and could benefit from the dispatchable load of a regional reverse osmosis (RO) facility and can process the regional system concentrate. Selection of the most cost-effective technology is needed to optimize the design and maximize economic value.

The INL study investigated the economics of blending a fraction of the regional brackish water to offset a corresponding amount of effluent water that is currently purchased from the city of Phoenix to provide reactor cooing. Due to constraints that limit the concentration of select water constituents in the Palo Verde cooling water, the economics continue to favor the use of effluent. Consequently, the assessment then considered the integration of the regional RO facility and a supplemental treatment process at Palo Verde to manage the regional concentrate to provide an alternative water supply to the surrounding municipalities (see Figure 5). The economic assessment considered the market value of the potable water and the benefit of concentrate management in this area. Also, the study included an assessment of the potential to run the regional RO as a flexible load to absorb some of the electricity price volatility at the APS electricity trade hub.

A developed water market model for the area suggests that large regional ROs (beyond 11000 AF/yr) will be most profitable. However, to dispose of the concentrate of larger regional ROs at the Palo Verde Generation Station (PVGS), additional evaporation ponds will have to be constructed.

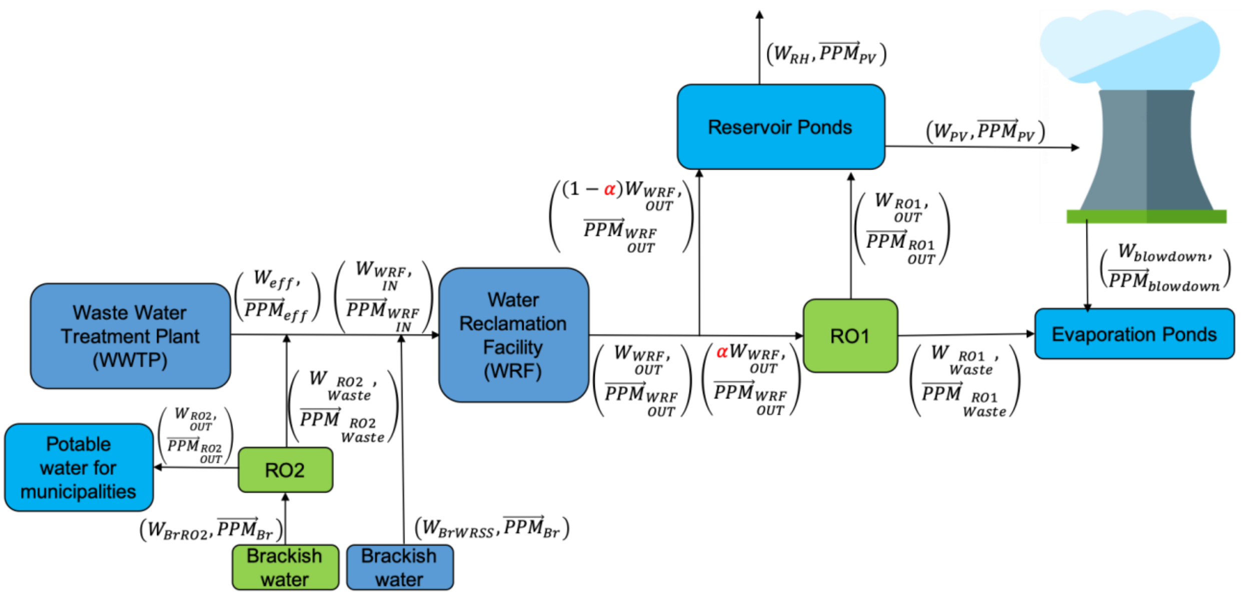


Figure 5. Effluent brackish water is pumped from the ground. Some of the brackish water is purified and sold (RO2), while the waste and some of the brackish water is blended with the effluent from the city of Phoenix' wastewater plant. This mix needs to be treated in an onsite RO (RO1) added to the WRF.

Future Work

There are several processes that have been demonstrated (outside IES) for producing clean water from saline rich water (either brackish or saltwater); however, global experience is dominated by three primary processes: two distillation-based technologies—multi-effect distillation (MED) and multi-stage flash (MSF)—and one membrane-based technology (RO).

A key distinction in the two methods is the way that they couple with a power source. The RO plant has the most straightforward coupling since it can operate using only electricity, which is needed to run the high-pressure pumps. Therefore, it is not essential to co-locate the desalination plant with the power plant so long as a grid connection is available. However, there may be an advantage for co-location of the power and RO desalination plant in terms of shared infrastructure and protection against grid disruption. Also, low-grade steam or warm wastewater from the power plant can be used to preheat the saline feedwater of the RO plant to improve its clean water production efficiency, although the quality of the distillate maybe adversely impacted.

Both MED and MSF plants require a thermal heat source such as a steam line from the secondary side of the nuclear power plant (NPP). For NPPs, this steam would typically be extracted via either the high-pressure or low-pressure tap on the turbine. Since energy quality requirements for MSF and MED are low, extraction from a low-pressure turbine stage could make sense. For space constrained power plants or steam cycles that preclude such integration, it is possible to take the higher quality steam from the steam generator through an already existing bypass valve and use higher quality steam for distillation processes.

Several factors are needed to understand the potential cost of potable water produced through a coupled nuclear-desalination process: energy requirements of the desalination processes both thermally and electrically, the cost of that energy, and the cost of the integration between the nuclear plant and the desalination process.

Also, the APS case only considered LWRs producing water for electricity market arbitrage using RO technology. Gaps within the IES program are to evaluate different markets for water desalination, different reactor technologies, and desalination technologies. In particular, nuclear waste heat utilization with heat-driven desalination techniques may be economically attractive. While heat-driven desalination techniques are usually economically inferior to RO, as part of an IES, they will allow for a better overall energy utilization (nuclear waste heat) and support social justice by producing water for communities.

2.1.2 Electric Energy Storage

Electrical storage (ES) is used in most current IES analyses as a baseline technology for comparison to TES. Because ES is only coupled electrically, there is no specific advantage of ES introduction to a grid as part of a thermal IES as opposed to decoupled on the grid generally. Thus, we expect the integration effects of TES to outweigh the benefit of decoupled ES systems.

Existing studies performed under the Light Water Reactor Sustainability program (LWRS) included lithium-ion battery storage as ES [8], generally with higher capacity costs but also higher round-trip efficiency when compared with various TES technologies. As expected, optimal results minimized the installation of ES for two reasons. First, the direct coupling offered for TES of lower capital costs means that if introducing energy storage is valuable in a system, TES will be preferred over ES. Second, the opportunity for profit via arbitrage was limited in most cases analyzed, which means profitability added by introducing energy storage is insufficient to recover capital installation costs.

Future Work

There has not been significant work in exploring a variety of ES technologies in studies under IES, largely because of the decoupled integration nature of the technology. If there are emerging technologies with lower capital cost for installation, there may be benefits to including details for those models in our framework. Additionally, future analysis on a sub-hour level may require the technical limitations of ES to be explored in more detail.

2.1.3 Thermal Energy Storage

The IES program has evaluated TES systems in support of the current fleet of NPPs as well as advanced NPPs (A-NPPs), with a focus on accommodating flexible power generation across multiple energy markets. A key component of these recent research efforts is exploring how nuclear energy can be used for purposes other than traditional electricity generation. A-NPPs may be tasked to operate in environments in which flexible power generation is more valuable than baseload generation. TES systems would enable NPPs to nimbly respond to market variability and could also enable A-NPPs to participate in multi-commodity markets, thus enhancing their economic competitiveness. While TES technologies afford a unique opportunity, the applicability of these systems is complicated by the fact that various types of NPPs are designed differently, each with its own temperature range, size, and operating fluids and conditions. Figure 6, which shows an example of a thermally coupled IES, represents one possible IES architecture. In a thermally coupled IES configuration, the nuclear reactor provides baseload heat or power and operates at a high-capacity factor to cover operating and capital costs. TES is used to attenuate the dynamics of subsystems or defer energy delivery to a later time. This enables the reactor to operate at or near steady-state design conditions, enhancing performance and minimizing maintenance costs. Depending on the amount of heat dispatched to thermal storage, the amount of power generated from the balance of plant (BOP) can be ramped up or down, thus allowing for flexible generation. Heat recovered from storage can be used either directly and fed to the power generation cycle or sent to an industrial process when coupled within an IES. Note that this configuration represents one possible scenario, and that the specific need for and potential benefits of energy storage may differ in other IES architectures.

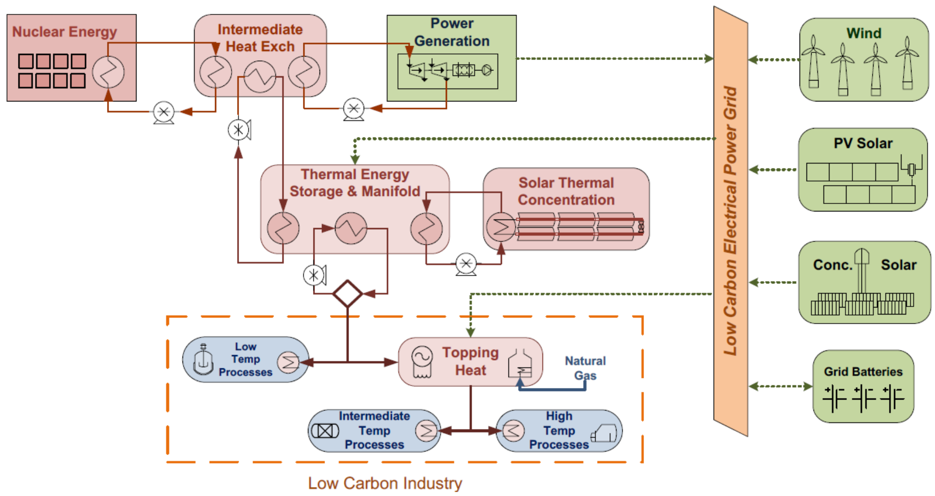


Figure 6. General architecture for a thermally coupled IES [2].

Work to date covered and explored the possibility of integrating a wide variety of TES technologies with various categories of NPPs, based on their individual operating characteristics. The full evaluation can be found in [9]. Two-tank molten-salt, solid-media, and latent-heat TES systems were deemed well suited for coupling with a wide range of advanced NPPs (A-NPPs) featuring different reactor sizes and temperatures. These findings, coupled with previous work in the field [10, 11], provide the starting point for a more in-depth analysis. This work created a database of current advanced reactors, leading to the development of an NPP classification tool for mapping A-NPPs to candidate TES technologies. This NPP classification tool was based on collected public information regarding all A-NPPs featuring adequate supporting data on their operations. The tool documents the reactor developer name, country of origin, licensing status, and design reference for each. It takes the form of pivot tables that filter the overall reactor database and categorize them based on their operating conditions (e.g., size, outlet temperature, pressure, and thermal efficiency) and other filtering criteria such reactor type, neutron spectrum, readiness to build, etc. In summary, the tool serves as a database, filtering, and classification tool in a manner useful for IES. Building from the Phenomenon Identification and Ranking Table and the figure of merit (FOM) study completed in Summer 2019 [12], the methodology explained in that study was applied to investigate advanced reactor designs alongside the current suite of proposed energy storage technologies. The evaluation criteria were as follows: technology readiness level, temperature compatibility, energy density, size, cycle frequency, ramp time, realignment frequency, geographic needs, environmental impact, and interventions. By combining the Phenomenon Identification and Ranking Table results and the classification tool described herein, users can determine the optimum TES technology by comparing the FOM results against the type, temperature, and size of the reactor of interest.

On the simulation and modeling side, work to date covered different options for coupling TES systems to A-NPPs in order to enable flexible and hybrid plant operation. An advanced LWR (A-LWR), high-temperature gas-cooled reactor (HTGR), and sodium-cooled fast reactor (SFR) were selected as the initial use cases for demonstrating a thermally balanced energy storage coupling design for thermal power extraction. Cost functions for the different reactor types were derived from fully balanced steady-state models developed based on three different coupling options having three different thermal energy bypass ratios. The models described the optimal deployment methodologies for achieving steady-state operation with minimum disruption to the nuclear power generation cycle. Then, the steady-state models and cost functions were used as a baseline to evaluate the transient controls and grid-wide economics for each coupling design and the techno-economic viability of such systems. This includes the analysis of the dynamic operation and process optimization by using the FORCE tools to evaluate the techno-economic viability and transient operations of TES-coupled A-NPPs using HYBRID and HERON. A detailed integrated setup of this kind, which includes steady-state models, transient-state, and techonomic analysis, would enable optimum energy storage strategies during periods of oversupply, dispatching it to produce electricity during periods of high demand or for use as heat by industrial users.

Future Work

Investigation of additional nuclear to TES coupling approaches: Future work will focus on technical approaches for achieving much higher temperatures from thermal storage (500 to 750°C) with advanced reactors, which opens up possibilities with various industrial users to meet their thermal need and electricity need. Current work on advanced reactors (LWR, HTGR, and SFR) focused on the use of heat from the steam leaving the steam generator as the source of heat for thermal storage. The challenge with such approach is that the maximum heat storage temperature is limited by the saturation temperature of steam at a given pressure, regardless of the initial temperature of steam leaving the steam generator. During the heat exchange process between steam and the storage material in heat exchanger, the majority of heat transfer occurs at the steam saturation point which is often much lower than the initial temperature of steam. This leads to lower thermal storage temperatures and, hence, lower heat quality during heat dispatch or lower thermal-to-electric conversion efficiency during TES discharge. In some reactor technologies, a more efficient thermal storage approach can be realized by avoiding this type of two-phase heat exchange process to achieve much higher thermal storage temperatures. HTGR, SFR, and Molten Salt Reactors (MSRs) that use molten salt as part of their reactor cooling system can be more forgiving if the molten-salt coolant loop itself is utilized as the heat source for TES rather than steam. Such approach requires that the heat for thermal storage be diverted from the reactor molten-salt loop directly rather than the steam generator.

Investigation of additional technologies: TES is generally categorized as sensible heat, latent heat, and thermochemical. Current use cases were focused on sensible heat storage. Although promising in terms of storage performance, thermochemical and latent heat are still primarily in the research phase of development having largely been relegated to laboratory experiments. To be employed in IES, additional research to design, demonstrate, and scale up these technologies is still required. The most common sensible heat technology is a two-tank system that utilizes either molten salt or thermal oil. This technology is currently being evaluated under the TES use cases from a techno-economic standpoint, physical responses within IES, and technical viability and is available as part of the HYBRID repository, a library of systems models developed in Modelica. In future use cases, additional sensible heat storage technologies will be evaluated, including rock or sand thermal storage, and concrete TES. These technologies are commercially viable and are promising options for evaluation as in context of nuclear IES. Latent-heat storage is also promising and was deemed well suited for coupling with a wide range of advanced NPPs and will be part of future use cases.

Investigation of refined cost models: While thermal storage will be a key component in IES as both a buffer between processes and as a contributor to the electricity market, it is vital to accurately evaluate both capital expenditures (CAPEX) and recurring costs such as Operation and Maintenance (O&M) cost of a TES technology. Currently, the CAPEX of various components required to design the TES in IES were acquired using the latest publicly available data obtained from Aspen Process Economic Analyzer (APEA V11). In addition to CAPEX, the following cost elements are typically captured from APEA: piping, civil, structural steel, instrumentation, electrical, insulation, and paint. While we found most of the costing data to be mostly accurate (i.e., in line with other data in literature), future efforts will focus on finding additional resources to refine our costing data and CAPEX estimates further. While a more refined and alternative plan has not been identified yet, this may include collaboration with partners in the industry and direct communication with manufacturers and vendors for the main components that are necessary for integrating a given TES technology.

Investigation of additional markets: The current TES use cases were focused on evaluating the capability of IES-coupled TES systems to act within the grid as a load response or equivalently as batteries in a given market or region (often selected based on market data availability). While this provides value and an overall baseline on the viability of a given TES technology, not all electricity markets reward these services. In future work, efforts will be made to review the different TES uses under different markets in the United States and generate a document that can be used as a reference to initiate a techno-economic analysis in the context of several U.S. markets, rather than a small subset or region. This will require the collection of additional information on market structure and the characteristics (e.g., ramp rate and duration) required to qualify for the market and, if available, impact of incentives or potential regulatory aspects that govern each region.

2.1.4 Nuclear Chemical Pathways

The nuclear chemical pathways consider carbon conversion pathways as an initial priority. The Carbon Conversion Refinery is a systems integration project focused on creating a closed-loop carbon refinery to convert coal feedstock into non-fuel products and capture and utilize CO_2 released from the intermediate processes. The final products of the refinery are chosen based on technical and market analysis. This project focuses on non-fuel products including chemicals, minerals, pure carbon products, and polymers. Pyrolysis of coal produces the syngas and solid feedstock used by the refinery, and tar and pyrolysis oils are converted to syngas via hydrothermal gasification. The processes within the refinery rely on nuclear heat and electricity and hydrogen from electrolysis. The production of hydrogen from nuclear and renewable energy sources and the use of nuclear heat eliminate most CO_2 output from the supply chain of the refinery products.

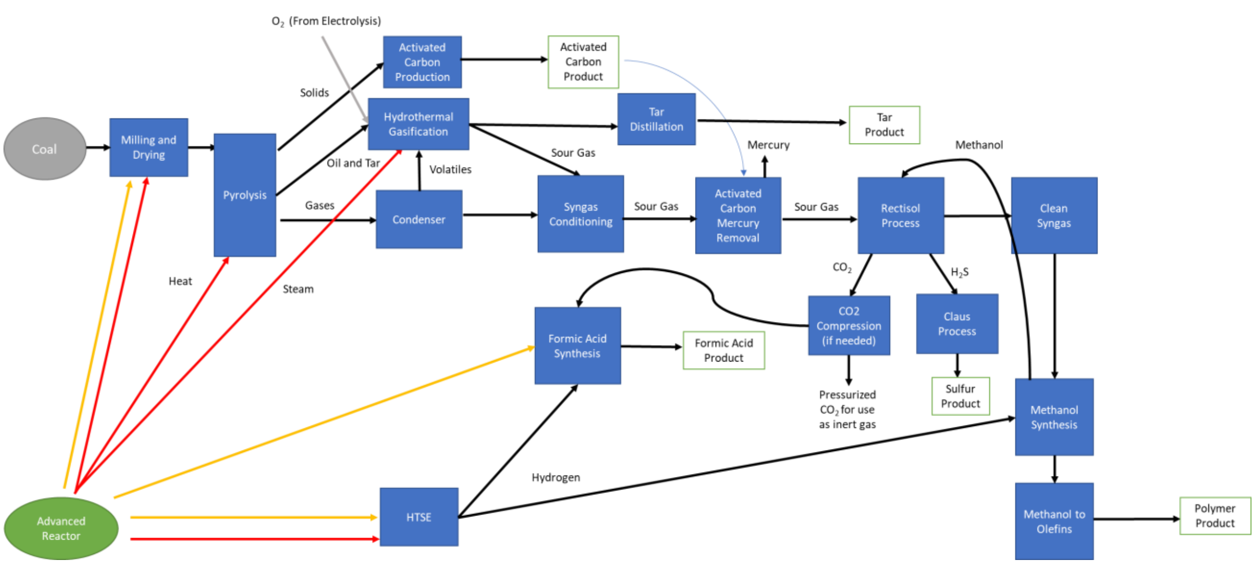


Figure 7. Flowsheet of the “carbon conversion refinery” design.

The modeling of these processes is intended to be flexible, so that the end products can change while keeping the main processes constant. For this reason, methanol was chosen as the downstream product of syngas. Methanol can be synthesized into chemicals as well as fuels, and could be easily replaced with a Fischer-Tropsch model while utilizing the same carbon capture and utilization strategies.

The cornerstone of the refinery design is carbon capture and utilization. While strategies to sequester compressed CO_2 are useful for mitigating climate change, carbon utilization strategies potentially increase revenue to the refinery and replace products traditionally obtained through a heavily carbon-emitting supply chain. Table 1 summarizes the products considered at the carbon refinery based on their technical readiness and market value. Formic acid is a simple product to integrate because it can be synthesized using captured CO_2 and hydrogen from electrolysis. However, it does not have as concentrated market value as urea, for which a switch to a non-carbon-emitting supply chain would have cyclical benefits if this fertilizer were used to grow biomass for sustainable fuels. Both urea and formic acid are of great interest to this project.

Table 1. Products considered for carbon utilization at the carbon refinery.

Product	**Technical Readiness**	**Additional Non-catalytic Inputs Required**	**Market Analysis**	**Choice**
Formic Acid	Commercialization in progress	Hydrogen	Steady demand across many industries	Good match for carbon refinery
Acetic Acid	Lab-scale processes only	Methane	Growth expected at 5.2% CAGR; China is largest market	Poor option because of lack of commercialization
Formaldehyde	Lab-scale processes only	Hydrogen	North and South America make up 10% of global consumption; Growth expected at 5.7% CAGR	Poor option because of lack of commercialization
Urea	Well-established technology	Ammonia	Steady growth for agricultural applications	Potential match for future analysis

Hydrogen produced from nuclear heat and steam is a particular focus of this design, and the scaling up of hydrogen production is expected to reduce the burden of capital investments that tend to exclude electrolysis substitution in plants that utilize natural gas-derived hydrogen, such as the ammonia and fertilizer industries. Alternatively, the investment into hydrogen from electrolysis at the carbon refinery can replace the water-gas shift for syngas, assist with carbon utilization processes, and potentially be sold as a pure hydrogen product on separate markets.

All reactor designs are considered for integration with the refinery. The use of existing nuclear infrastructure would help make plants more profitable and reduce the capital costs of building a carbon refinery. It would, however, require either an all-electric steam generation system or significant changes to the plant design to obtain process steam.

Advanced light-water and high-temperature reactors are both suitable for the refinery as well, although a low-temperature reactor would require heat augmentation to satisfy the process requirements. Figure 8 summarizes some of the process requirements for the refinery and the steam supply characteristics of some advanced reactors.

The feasibility of the refinery will be evaluated by comparing the carbon output and Net Present Value (NPV) of the refinery to incumbent technologies that produce the specified end products. These scenarios will also help to determine the value of the carbon utilization market as an alternative to carbon sequestration.

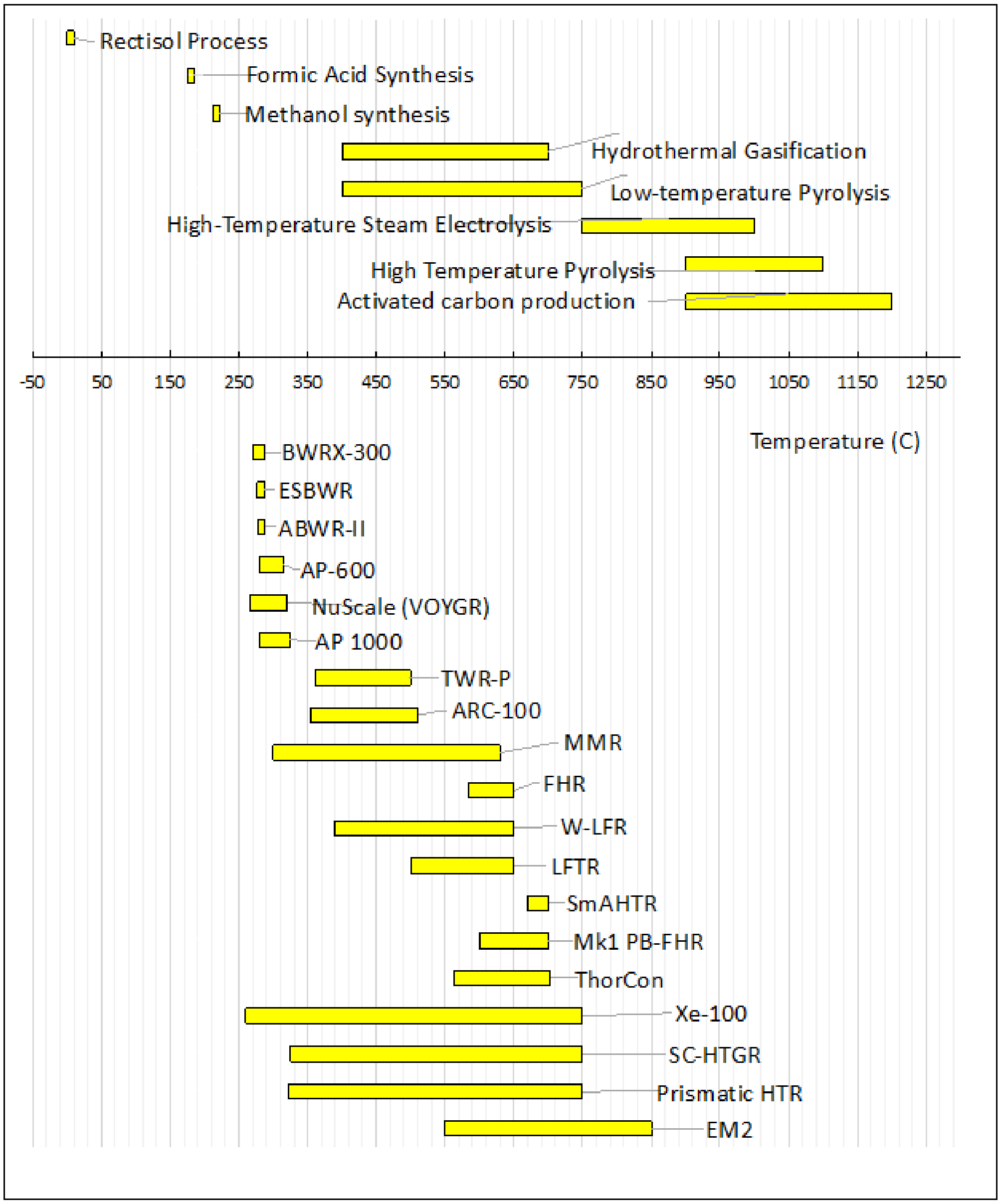


Figure 8. Summary of carbon refinery process requirements and advanced reactor design steam supply quality. Heat augmentation might be required to match reactor to process. (From top to bottom: Boiling Water Reactor X-300, Economic Simplified Boiling Water Reactor, Advanced Boiling Water Reactor II, Advanced Passive PWR (AP-600 and AP-1000), Traveling Wave Reactor-Prototype, Integral Fast Reactor (ARC-100), Micro Modular Reactor, Fluoride Salt-Cooled High Temperature Reactor, Westinghouse Lead-Cooled Fast Reactor, Liquid Fluoride Thorium Reactor, Small Modular Advanced High Temperature Reactor, Mark 1 Pebble-Bed Fluoride-Salt-Cooled-High-Temperature-Reactor, Hybrid Thorium Unranium Liquid Fuel Molten Salt Small Modular Reactor (ThorCon), X-Energy 100, Steam Cycle High-Temperature Gass-Cooled Reactor, Prismatic Modular High-Temperature Gas-Cooled Reactor, Energy Multiplier Module)

Because of the complexity of this system, there has been a significant amount of literature review and decision-making required to determine the processes, components, and markets to integrate for the optimal design. The next step is creating the static model of the chemical processes using Aspen HYSYS. This will allow the team to evaluate the economic performance of the refinery and make changes to the potential markets. This will lead to the dynamic modeling of the plant and determination of storage opportunities to extract higher value from certain markets. The team will also explore scenarios which continue to reduce carbon output but lower capital investments of the complex refinery. This includes outsourcing downstream production of methanol derivatives to existing plants or insourcing ammonia from a local plant which is utilizing hydrogen from low- or non-carbon-emitting sources for fertilizer production. These collaborative scenarios are particularly aligned with the goal of the project to maintain local economies by transitioning to nuclear heat and steam over fossil fuels.

Future Work

The modeling flexibility of this system will allow for a variety of cases to be explored in the future. Specifically, future carbon conversion cases will be focused on producing ammonia, urea, and other fertilizers. As the world's population grows, demand for fertilizers to grow more food will continue to increase. Also, regulations on biofuels that require the feedstock supply chain to be decarbonized will introduce new demands for zero or low-carbon generated fertilizers. Nuclear steam and electricity will be vital to generate hydrogen for this purpose. Urea is also a beneficial fertilizer because it is produced by combining carbon dioxide with ammonia, and its production can therefore be carbon negative.

The conversion of coal to carbon-based products with minimal production of carbon dioxide is an important process in the transition to a decarbonized future because we will still need the chemicals and materials derived from coal and other fossil fuels until a better alternative is proposed. In the future, a similar approach could be taken to convert natural gas and oils to non-fuel products as well. At present, this is not an efficient conversion compared to the direct use of these fuels, but if carbon taxes or other regulation reduce its use worldwide, they may be more viable as carbon feedstock. As fossil fuels continue to play a large role in our energy infrastructure, we must find new ways to utilize them without the negative environmental effects of fuel combustion.

2.1.5 Synfuel Production

Over the past decade, INL has completed and/or supported several synthetic fuel production analyses. The earliest analyses performed during this period were performed for the Next Generation Nuclear Plant (NGNP) program and were focused on steady-state applications using coal and/or natural gas as the carbon feedstocks. Specific analyses included the Nuclear-Integrated Methanol-to-Gasoline Production Analysis [13], the HTGR-Integrated Coal and Gas to Liquids Production Analysis [14], and the Nuclear-Integrated Methanol-to-Olefins Production Analysis [15]. While the methanol-to-gasoline and coal/gas to liquids analyses (based on diesel production via the Fischer-Tropsch [FT] pathway) developed chemical process models that continue to be relevant for current and future synfuel analyses, the reactor costs, synthetic fuel prices, and carbon feedstock sources considered in these analyses are dated and would need to be updated if the results of these analyses are to be considered in the current technology and market environment. The methanol-to-olefins analysis considers production of synthetic ethylene and propylene chemical products and therefore does not provide results that are directly applicable to synthetic fuel production applications.

In Fiscal Year (FY) 2020, INL subcontracted Pacific Northwest National Laboratory (PNNL) to perform an analysis comparing two possible synfuel production routes utilizing CO_2 as the feedstock [16]. The analysis considered an NPP with energy output and cost characteristics representative of the current fleet of LWRs as the basis for providing energy input to the synfuel production processes. The analysis considered CO_2 from bioethanol plants in the vicinity of the LWR as the source of the carbon feedstock. The study evaluates co-electrolysis of CO_2 and water to produce syngas that is converted to synfuels in subsequent process steps. The study investigated both methanol and ethanol pathways for synfuel production. The results of this study justify further pursuit of synfuels via the methanol-to-fuels as an alternative market for LWR energy use. The synfuels could be competitive in price with petroleum fuels if credits for CO_2 emissions reductions become available or if the price of petroleum fuels rises above historic lows that existed when this analysis was performed.

In FY-22, INL and Argonne National Laboratory (ANL) collaboratively evaluated synthetic hydrocarbon fuel production via the FT reaction. The FT process typically produces a mixture of naphtha, jet, and diesel fuel referred to as FT fuels. ANL reports [17, 18] provide techno-economic analysis of a steady-state FT process coupled with LWRs, which provide heat and power for hydrogen production using high temperature steam electrolysis as well as electrical power for the FT process. The CO_2 feedstock cost is based on the compression and transport costs from nearby corn bioethanol plants. FT process models were developed at three scales of NPPs: 100 MWe, 400 MWe, and 1000 MWe.

The economic analysis of FT fuels compared the synfuel minimum fuel selling price (MFSP) with historical diesel fuel prices. The analysis concluded that the FT fuels cost of production is mainly driven by the H_2 price. With an H_2 cost of $2/kg and a CO_2 cost of $25/MT, the production cost per gallon of FT fuels in a generic location is estimated to be $4.04, $3.42, and $3.27 for the three NPP scales, respectively. This hydrogen price results in a FT fuel MFSP similar to the diesel 15 year high price for the 100 MWe NPP, and an FT fuel MFSP lower than the diesel 15 year high price for the 400 MWe and 1000 MWe NPPs. If the hydrogen price is reduced to $1/kg, the FT fuel MFSP is similar to the diesel 15 year average price for the 100 MWe NPP and the FT fuel MFSP is lower than the diesel 15 year average price for the 400 MWe and 1000 MWe NPPs.

The INL and ANL FT fuel analysis will continue to evaluate FT fuel production for a dynamic operating mode into FY-23. The dynamic synfuel production operating mode allows the NPP to dispatch electrical power to the grid or to the synfuel production application depending on market pricing signals. Hydrogen storage will be considered to enable the dynamic dispatch of the NPP while allowing the FT process to continue to operate under steady-state conditions. HERON will be used to determine the optimal FT plant and hydrogen storage capacities as well as determine the dispatch schedule that maximizes the NPV for selected FT fuel production case studies.

Future Work

Synthetic jet and diesel fuels provide significant opportunities for decarbonization of transportation sector (e.g., heavy transportation applications such as truck, rail, aviation, and marine). Therefore, analysis of synfuel pathways that prioritize jet and diesel production should continue to be emphasized in the future. Operation of synthetic fuel production processes in grid-integrated schemes and integration with small modular reactors (SMRs) may provide opportunities to decrease synthetic fuel production costs while also contributing to grid reliability. Future synthetic fuel modeling and simulation work should continue to investigate synfuel production pathways that have characteristics that will allow decreased fuel production costs through decreased hydrogen usage, ability to operate in grid-integrated applications, and/or ability to operate at the scale necessary to minimize feedstock costs and integrate with SMRs. Therefore, continued work is necessary to perform techno-economic analysis of additional synfuel production pathways and provide a decisive basis for identifying and selecting the synfuel production technology with technical and economic characteristics best suited for nuclear-based synfuel production.

The current approach for dynamic FT process operation involves transient hydrogen production and storage with steady-state operation of FT reactor and downstream operations. Since hydrogen storage is expensive and/or energy intensive, investigation is necessary of reactor types (e.g., microchannel reactors/microstructured, packed bed reactors) that allow dynamic production of FT synthetic crude products and/or synfuel production pathways different other than FT that allow production and storage of different intermediate chemical compound (e.g., methanol, ethanol, and dimethyl ether [DME]). Evaluation of the cost benefits of being able to dynamically produce synfuels without the requirement to storage hydrogen will require process and dynamic model development/updating prior to performing dispatch optimization analysis to evaluate process economics.

In addition to the FT process, candidate synfuel production pathways for producing jet and diesel fuels include methanol-to-olefins to gasoline and distillate (MTO/MOGD) and DME production processes. The MTO/MOGD process product slate can be tuned to produce large fractions of diesel fuel. DME can be produced from methanol and could be used as an alternative to diesel fuel. Both pathways produce methanol as an intermediate product, which has advantages for dynamic methanol production and intermediate storage in grid-integrated scenarios. Development of Aspen Plus and Modelica models is necessary to fully evaluate these pathways through calculation of process mass and energy balances, capital and operating costs, as well as transient operating characteristics. Availability of a “price-maker” (e.g., large enough that decisions impact market price) dispatch analysis toolset would enable more realistic modeling of large-scale grid-integrated production cases. Incorporation of SMR performance and cost attributes into synfuel TEAs will provide insight into how SMR reactor technology could best be utilized to provide increased nuclear power generation resources for synfuel production (e.g., smaller-scale local/regional synfuel fuel production may benefit from reduced feedstock [CO_2] and product transportation costs relative to large-scale production cases, construction of new SMR units may enable dedicated nuclear synfuel production plants with simplified steady-state operating modes). Finally, aligning modeling and simulation efforts with projects and/or collaborators performing experimental evaluation and/or demonstration of the various synfuel production pathways considered will provide opportunities for validating the design basis and performance estimates of the synfuel production models. Demonstrations of coupled processes (e.g., hydrogen production coupled with synfuel production) will provide the greatest opportunities for validating model predictions.

Due to the decreased life-cycle emissions of low carbon, drop-in synthetic transportation fuels relative to conventional transportation fuels, low-carbon synfuels will likely be treated by transportation markets as a different product from conventional fuels. Therefore, evaluating the economic viability of synfuel production by comparing the synfuel production cost with the cost of conventional petroleum-based fuels may not be the most applicable approach. Therefore, economic models and/or the approach used for economic analysis of synfuel production must be updated to allow the comparison of synthetic fuels produced via nuclear-based pathways with low-carbon footprint synthetic fuels produced using other pathways, such as sustainable aviation fuel made from renewable biomass and waste resources as well as drop-in synthetic fuels produced using renewable energy.

2.2 Experiment Demonstration Support and Control

Once technologically and economically viable use cases have been identified in the techno-economic analysis, experimental demonstrations with modeling and simulation support starting at lab-scale experiments going to full-scale commercial integrations can begin. The modeling and simulation needs for experimental support are grouped in three areas of interest: advanced monitoring and autonomous control of IES via DT, technology scaling, and model validation.

2.2.1 IES Control via Digital Twins

A fully functioning DT consists of the physical space, its representation as a computational model (physics-based, data-informed, ML/AI, etc.) (i.e., the digital space) data flowing from the physical system to the computational model, and data flowing back from the computational model to the physical system (i.e., data space), and finally the services, recommendation, and capabilities offered by the DT and complying to the customers’ requirement (i.e., services space) as depicted by Figure 9 [19]. A DT is most useful if data flows in both directions. Data flowing from the physical system to the computational model is used to update or calibrate the computational model to perform a task like decision-making, optimization, or control. Data flowing back to the physical system from the computational model is used in the real world to update set-points, inform operators of the health of the system, perform autonomous control, and/or detect anomalous operational behaviors in the physical system.

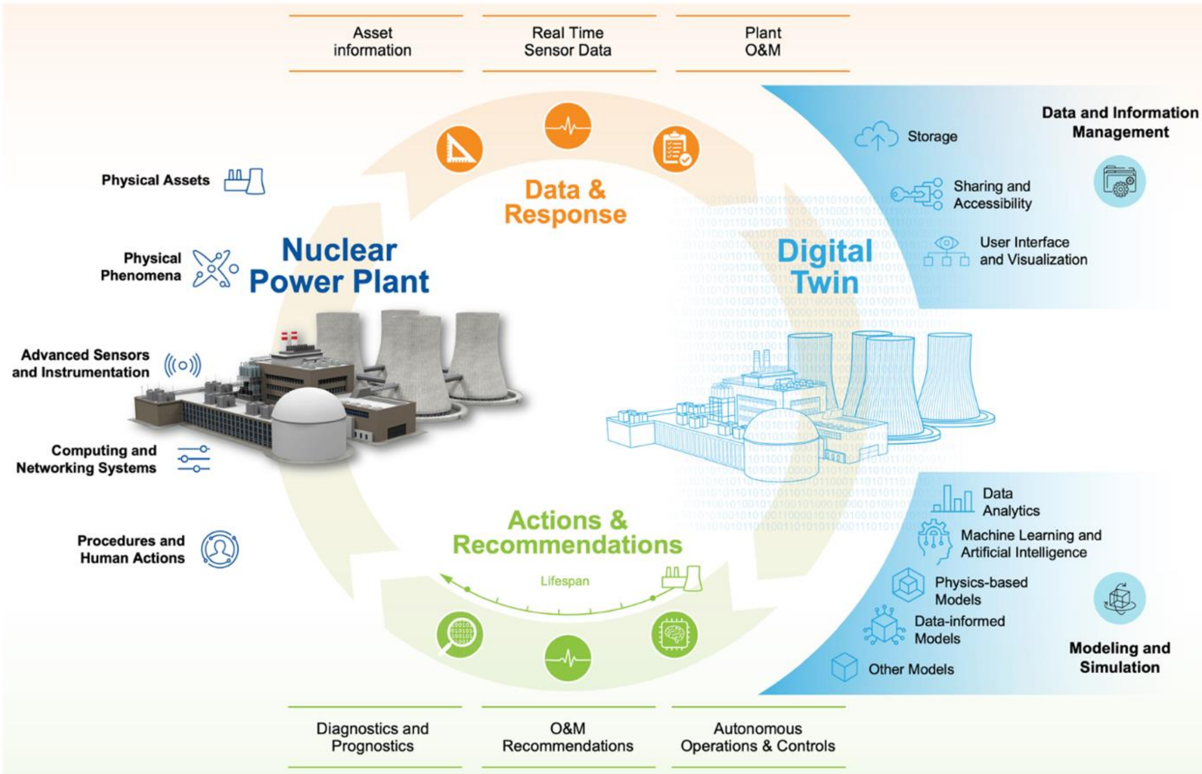


Figure 9. The four spaces of digital twins (figure from [19], p. 2).

Storing and retrieving physical system data and computational model data are of utmost importance for a successful DT deployment. DT data must be stored in a digital, structured, scalable, secure, and centralized environment. Data handling solutions must ensure that data can be accessed in real time across decentralized users, DT models, and physical system data storage. In addition, a user interface is required for an operator to interact with the DT system. For the IES-DT work performed at INL, the current data storage and handling solution is the DeepLynx data warehouse platform currently under development. DeepLynx is specifically designed for nuclear applications, and IES will adopt it when it reaches sufficient maturity and flexibility to be integrated. In the meantime, existing commercially available data warehouse platforms including Microsoft Azure, Amazon Redshift, Google BigQuery, or Snowflake, should be investigated to determine the optimal data warehouse solution for IES-DT applications.

DT computational models can come from many sources including physics-based, data-informed, or ML/AI. Key challenges for DT computational models include uncertainty quantification (UQ), verification and validation, and model integration. Current IES-DT model development is based on training ML/AI models on data generated by Modelica models coming from HYBRID. Work to add additional model components in HYBRID is ongoing. Training ML/AI models on the Modelica models allow the models to run much faster and be used for decision-making in DT workflows. DT models could come from other sources, including Functional Mockup Interface / Unit (FMI/FMU) or experimental data; future work could address these types of models.

Currently, work in the RTO area is focused on demonstrating the software capabilities that will enable future DT demonstrations on physical systems. The computational models used in RTO workflows consist of trained RAVEN ROMs from HYBRID Modelica models. These RAVEN ROMs are augmented as grey box models which include additional information about the model itself (metadata), such as Jacobians and other derivatives; as such, grey-box models are in between "black box" models, where the input/output relationship is not extractable from the model, and "fully transparent" models where analytic forms of the input/output relationship are available. Grey box models allow integration with the optimization package Pyomo to perform real-time economic dispatch optimization. Without the grey box model, optimization is limited to black box optimization routines which traditionally take too long to find an optimal solution to run in real time. Smaller-scale electric energy storage models have been used to demonstrate the purely software side of an optimization workflow running in real time for a DT.

Future Work

Future work in the RTO area will include integration with the Dynamic Energy Technology and Integration Laboratory (DETAIL) to demonstrate the software and hardware capabilities required for a fully operational DT workflow. The primary challenge will be setting up the data storage and handling platforms. The reason is that while lots of these data warehouses claim real-time transactions, the definition of 'real-time' varies from one platform to another. Furthermore, these data hubs require knowledge of Structural Query language (SQL) and its modern alternatives (NoSQL and NewSQL). Once the data storage and handling platform is set up, additional challenges remain in treating real-world data that can be noisy or missing. The computational models for DETAIL can come from Modelica models in HYBRID or experimental data. Investigations of the benefits of each approach with regard to computational speed and accuracy will need to be performed.

Many areas of DT work within IES remain to be explored. Optimization, system health monitoring, reliability, cybersecurity monitoring, and other real-time workflows can be demonstrated on DETAIL or other physical IES. Coupling multiphysics models or multiple components will need to be demonstrated. DT demonstration projects with commercial, state, or municipal partners will advance net-zero goals and improve IES system operations in real time.

Several modeling and simulation characteristics can be indispensable for achieving real-time accurate replication of the physical assets and processes and supplying educated predictions, suggestions, recommendations, and even prompt actions to avoid accident scenarios. Some of these characteristics are described below.

One example of a necessary M&S characteristic is optimal data query (in terms of time, instrumentation types, and location). Cutting-edge algorithms have proven that more data is not necessarily better data; in other words, forecasting demand, loads, prices, and weather are vital for IES and solely drives the dispatching decisions. Deciding when and where to collect the data to avoid outliers, false dips and/or spikes, noise data, and correlated instrumentation can be a game changer. Ongoing Laboratory Directed Research and Development (LDRD) efforts are trying to address such problems on smaller scale applications; nevertheless, the impact multiplies significantly for IES applications as the cross-correlation is not only between components but also between subsystems.

Another missing essential aspect is multiscale modeling and AI-based communication across different scales. While this might not be the primary focus of IES, each subsystem provides a continuum scale (system scale) as the dynamic simulator. If real-time adaptation is sought, finer scales should be available to explain changes that global effects might not be able to interpret or capture. There should be AI governors that decide based on robust metrics which scales should be hooked to the simulations and which ones should be unplugged. (This aspect has never been explored before and may be an avenue for future LDRDs until they become sufficiently mature to be adopted by the programs).

The next crucial gap is the lack of data, specifically historical data and the need for data synthesis. While there are some ongoing explorations to address this aspect, several alternative techniques should be considered to replace random data synthesis with physics-based data synthesis and rare-events data synthesis, etc. The problem with traditional data synthesis techniques is that these methods either add white noise to previously considered data or randomly alter some of the signal features. This leads to either repeating some training sites and hence giving these sites a higher probability of occurrence or creating non-physical signals. Moreover, such an approach will not capture any rare events and treat them as noise. To mitigate such a challenge, model-data synthesis should be considered.

Multi-resolution time series analysis can be a natural extension to the Time-Series Analysis (TSA) module in RAVEN to facilitate more advanced filters to the time series data, such as weather data, demand data, electrical load time series, etc. This can help filter out induced disturbances, background noise, outliers, among others. It can also be performed in frequency domains and render more stable transfer functions that provide better controllability.

Uncertainty propagation and prediction in ML models are other directions that should rise to the surface, as these contribute to the trustworthiness of digital replicas. While several ML/AI models offer uncertainty bands with no additional costs, such as Bayesian Neural Networks (BNNs), Gaussian Processes (GPs), and some variants of Dynamic Mode Decomposition (DMD), sometimes these models are not the predictors that accurately mimic the dynamics in-hand. In such cases, different treatments for the uncertainties are needed. This can be facilitated via inverse uncertainty analyses using Bayesian frameworks and Markov Chain models.

To add to the list, a large benefit can be gained from acquiring the capability of model assimilation and adjustment. This is used when a ROM is performing well and is validated by the streaming real-time sensory data, then a discrepancy starts to occur and the ROM predictions gradually drift away from the reality experienced by the physical asset. In that case, there should be a robust way to decide if the models should be retrained, adapted, retired, or even disconnected and replaced by another ROM from the ensemble of models prepared for all the scenarios anticipated from the dynamic system. The infrastructure to enable such capability is already in RAVEN's ensemble models, hybrid models, and logical models, but the metrics upon which the decisions are made are far from complete. The ability to retrain models, adjust weights and biases, or tune hyperparameters (used to estimate model parameters) in real time is a very attractive and promising solution to improve model robustness.

Data are not optimally utilized at present. For instance, operator logbooks are still relying on domain experts and are subject to human errors and delays. State-of-the-art treatment for such a different data type (text) is using transformer models with attention mechanisms; these models currently use solely data-driven methods to direct the AI's attention to important words and tie correlated phrases. If more physics insights are introduced to these attention models, this can revolutionize Natural Language Processing (NLP). Furthermore, data fusion techniques are being explored at INL to convert sensory numerical data to strings in order to aggregate them with text-based data from logbooks, literature, and the internet, then use NLP to learn from these data, link consequences to causes and hence offer better predictions, diagnostics, and prognostics. This can be applied on multiple levels: the component level, the subsystem level, and the integrated grid level.

The IES applications currently rely on the linear correlation between different components/events, whereas for proper governing, real-time decisions, and proper dispatching actions, all models should try to infer causality. If the root cause is identified, the action no longer relies on expert judgment and domain knowledge but rather is easily automated, and only then can real-time actions be achieved. Causal AI is a very rewarding discipline yet is in its infancy, and deeper research should be conducted in this direction. Bayesian Neural Networks are the natural evolution of traditional Neural Networks to propagate input uncertainties to the responses of interest, and, specifically, Directional Acyclic Graphs (DAGs) can serve to leverage the system models from Modelica and convert them to graphs where the nodes of the DAG graph are driving/primary model variables, and edges represent causal effects. This also will boost the data communication with DeepLynx as it strongly supports GraphQL; hence, communication protocols will be much faster and significantly more efficient.

The cyber resilience and anomaly detection components are the defense layer not only against cyberattacks but also against naturally induced anomalies caused by faulty instrumentation, noisy data, failed components, leakage, degraded components, etc. More algorithms/capabilities should be oriented towards such an evolving challenge.

Finally, to check all these boxes and still claim real-time operations that still offer all these capabilities, more cloud computing should be utilized. Currently, only data storage might utilize the cloud, but in a few years, IES DTs should utilize cloud computing, accelerators such as Graphics Processing Units (GPUs), Tensor Processing Units (TPUs), and maybe one day even quantum computing and quantum machine-learning.

The new design paradigm that DTs facilitate suggests different mindsets for physical assets that are not built yet, as well as revolutionizing what is already built. Once the IES-DT framework is ready, it should be able to cover the whole spectrum of applications from the DT prototype phase that initiates the virtual space and prepares it to realize the physical asset once it is up and running, to the DT instance which registers each physical asset once added to the grid, to the DT aggregate which combines all the component level DTs, unit level DTs, and system level DTs, to form the process level DT that comprises several systems until the retirement of components and even systems. Each thread of data collected from early design until retirement for a single source of truth (digital thread) can provide guidance for new applications. This should be able to offer capabilities such as decision-making with minimal-to-no human intervention and ultimately not only giving recommendations but also taking the necessary actions. It should be used in all aspects of energy production, plan monitoring, maintenance scheduling, energy storage, designing compact components, coming up with smart materials and additively manufactured parts, designing recoil networks to fool cyber-attackers, and deciding between up-scaling of current plants and building new ones with the appropriate size that smoothly integrates to the grid. The IES DT should be able to perform all economic modeling and compare different business choices to give the customer an educated recommendation with less uncertainty. It should be capable of adopting advanced reactors and next-gen technology by accommodating their new requirements. As giant tech companies bond together to form the ***Industrial Metaverse*** **[20]**, the IES DT should be the ***Energy Metaverse*** that offers a completely immersive experience.

2.2.2 Scaling

The IES engineering-scale setup at INL is a combination of thermal storage, battery testing, hydrogen production, electrical vehicle charging, a digital real-time power grid, distributed energy and microgrid, power plant operation, and a non-nuclear microreactor experimental testbed called DETAIL. The goal of DETAIL is to have each system communicate and emulate an IES environment [21]. This includes receiving external signals from industry utilities as inputs to enable real-time data-driven experiments. One component to consider is the design of the experiments when one DETAIL sub-system is interacting with another. Since each facility in DETAIL is an individual specialized group, the physical ties between the systems are not yet analyzed in detail, and for every new experiment design, the integral effects on all systems must be evaluated. Another component to consider is how to translate the industry data into lab configurations. Lab-scale facilities are downscaled versions of industry-scale power plants or energy processing utilities, and inputting raw data would not realistically match lab configurations. For this purpose, a data postprocessing step is required to convert output data into configurable input data in the correct sequence, based on physics (i.e., when industry-scale data comprise data points for every hour, each data point needs to be converted to correspond to a lab-scale data point). This can be accomplished by scaling the system, component, process, and/or closure relations if necessary to adjust the magnitude and series of more than two interacting (physically or virtually) systems. A successful scaling will achieve fully synchronous interactions among systems where output signals from one facility is postprocessed as input signals for another facility conserving the physics in the latter. Two scaling methodologies are considered in the IES program: DSS [22, pp. 219–260] and Hierarchical Two-Tiered Scaling (H2TS) [22, pp. 194–201]. DSS represents scaling for transient processes, and H2TS is the main tool for static scaling of steady-state and transient systems.

Current Work

As a demonstrating case to test both scaling methodologies and reconfigure data to desired settings (or data projection), the thermocline thermal storage system (TTSS) of the Thermal Energy Distribution System (TEDS) was selected. Based on flow conditions, geometry, materials, and transient behavior, the fundamental equations were determined and discretized to include TTSS inlet and outlet parameters [23]. The equations were non-dimensionalized separately according to the DSS and H2TS definition.

The first demonstration case consisted of understanding scaling distortions in TEDS when accelerating a TTSS draining transient to double its original speed. For DSS, as anticipated, the derived twice-accelerated case showed perfect scaling for the TTSS temperature distributions (overlapping of data is proof of ideal scaling) and demonstrated the data drift in comparison to the original dataset (using β−time representation). For H2TS, all mass, momentum, and energy characterized time ratios were matched well within a relative error of 0.01. The data projection was successful and provided a TTSS test that achieved the same energy charge and discharge in half the time.

While abiding by scaling restrictions, such as unchanged geometry and materials, the accelerated test was calculated by projecting the original dataset using the DSS and H2TS methodology. One of the unexpected yet significant findings of this scaling activity was that without the freedom to change the geometry of the system, the scaling ratios were only dependent on system properties (e.g., fluid density). The distribution of these properties varied from one to another and restricted the range of feasible scaling ratio values. The property limitations caused different effects for both scaling methodologies. For DSS, the coordinate transformation was confined to ω-strain, and other types were not feasible. For H2TS, although all characterized time ratios were matched, the momentum residence time could not be near 0.5 at the same time as the energy residence time was adjusted to be 0.5. This is an example of H2TS scaling distortions where some phenomena may be disregarded for conservation of others. For the comparison of both methods, DSS was capable of projecting the whole transient, and H2TS provided the reference data point. This is expected since DSS is a transient analysis method, and H2TS is static. For future reference, if more dramatic test acceleration were to be desired without varying geometry, a change in the fluid medium of the TTSS would have to be considered.

Another data reconfiguration demonstration case was conducted for the High Temperature Electrolysis (HTE) facility in DETAIL. To limit the analysis to hydrogen production, the physics occurring within the fuel cell was considered. The following solid-oxide electrolysis cell (SOEC) phenomena were scaled: stack voltage, overvoltage, and SOEC thermal dynamics. Similar to TEDS, DSS and H2TS were applied to achieve the scaling ratio and characterized time ratio expressions. Despite the absence of available data to test the scaled set equations, all preparations have been made to initiate data analysis.

Future Work

Following the work developed in FY-22, there are three priorities before initiating DETAIL and external facility real-time signal communications: scaling of other facilities in DETAIL, testing of the demonstrated cases, and emulation of IES in the engineering-scale. Although the partial scaling of DETAIL facilities has been conducted for TEDS and HTE, the scaling analyses of the coupled piping and other modules such as heat exchangers (HX), are necessary. When physically connected, the shared components (i.e., in the case of TEDS and HTE, an HX exists to supply thermal energy to the SOEC endothermic processes) can be scaled on either end (i.e., in the previous example this would be TEDS and HTE) to act as the common denominator to associate scaling ratios or characterized time ratios of one system to another enabling synchronized transient interactions (virtually connected systems will have sections that represent quantity in/out and will be scaled).

Testing of the scaling methodology for individual DETAIL facility components needs to be completed. The main motivation is to ensure the data projections are accurate enough for the cross-system interactions phase. The demonstrated projections based on previous data alone do not prove the newly calculated data to be true. There are cases where the modeled governing equations lack essential physics to correctly capture the evolving phenomena, or where inappropriate assumptions may have led to discrepancies. Two elements are required: the individual design/data of a consistent experiment for each DETAIL facility and running the projected experiment design to measure the scaling distortion.

Also, full IES emulation testing needs to be considered. The experiment design step will be relatively simple since prior scaling activities reveal dominant system, component, process, and/or closure relations. The vital aspect to the experiment design is arranging all systems to work synchronously guaranteeing time-dependent phenomena characterization in all participating facilities. The experiments should allow all DETAIL systems to run real-time if necessary whether connected physically or virtually (it is recommended to use RTO).

Furthermore, connecting DETAIL to external systems via input/output scaling needs to be demonstrated. None of the facilities built in DETAIL have a target system; rather, each represents a generic engineering-scale implementation of the existing technology. For adjusting inputs/outputs signals, the previous scaling acts as a model that can be quickly referenced to determine scaling ratios. Considering DETAIL is meant to become a user facility, this capability provides immediate feedback with thorough theory behind each analysis documented by milestone reports and publications. DETAIL should be able to accommodate the following user objectives: IES emulation, database for calibration and validation via scaled DETAIL generated data, and experiment optimization via engineering-scale testing. The full analyses should inform users which experiments to run and the associated boundary conditions to achieve the intended results. Also, if engineering-scale data can be converted to industry-scale (or vice versa), received external data can contribute to back-validating the developed models at INL. This includes the HYBRID suite as it will require data from users, economic cases from open sources, and a viable IES workflow to expose established code for demonstration and model validation.

One other potential development is to adjust the DSS methodology and associated code implementation so that it becomes applicable to model validation and verification (V&V) and UQ. Using the unique metrics provided by DSS, distortion can be measured for a given systems. The metric should be capable of conducting sensitivity analyses for various forms of perturbations applied to simulations and confirm input ranges that the code models are applicable for. The proposed development will have to derive a DSS-specific acceptance criteria based on statistics and/or differential geometry to determine the threshold of measured distortion and uncertainty. Coupled with the DOE-NE IES program, this new capability could be another service provided to future users.

2.3 Technology Interconnections

It is outside the scope of IES to design the heat/electricity producing plants (or they already exist) or the chemical processes involved in an IES. Rather, IES works to develop, evaluate or implement technologies that thermally connect different assets into an IES.

2.3.1 Heat Exchanger Optimization

HXs are one of the key components of IES for thermal integration of disparate energy systems, such as NPPs and industrial heat processes. HX development and application to IES, however, is still a challenge as multiple factors must be considered in heat exchanger design, including potential safety and operational issues inherent to IES. Given that the role of component technology such as the HX is critical to IES operation in coordinating the exchange of energy currency among multiple subsystems, optimal selection based on both cost and performance of the HX technology is an important part of IES research and development. Also, it is important to note that the decision on the optimal selection may vary depending on the heat exchanger’s application target (i.e., thermal systems to be coupled within an IES) and the associated end-user (i.e., customer) demands.

Currently, the IES program is working to establish a systematic methodology to support the optimal selection of heat exchanger technologies for IES, with a particular focus on thermal integration between advanced nuclear reactors and industrial heat processes. Figure 10 shows the overall logical decision path to determine the optimal choice of an IES heat exchanger among various alternatives, which indicates that the decision for IES heat exchanger selection requires three elements: (i) operational target, (ii) evaluation metrics, and (iii) decision-support matrix. To specify the operational target ([i]), a system-wide optimization, which determines optimal IES configuration and component sizing, etc., can be used to refine the heat exchanger's performance. For the evaluation metrics ([ii]), three types of high-level metrics are considered as inputs for the decision-support matrix: 'functional requirements', 'cost factors' and 'benefits and risk analysis' as shown in Figure 10. Then, more detailed (i.e., low-level) evaluation metrics are derived using the Analytical Hierarchy Process (AHP) technique for thorough comparison of all essential aspects of candidate heat exchanger technologies. Lastly, a decision-support matrix ([iii]) is created using the Quality Function Deployment (QFD) method to consider both end-user demands and associated technical requirements of heat exchangers through the evaluation process.

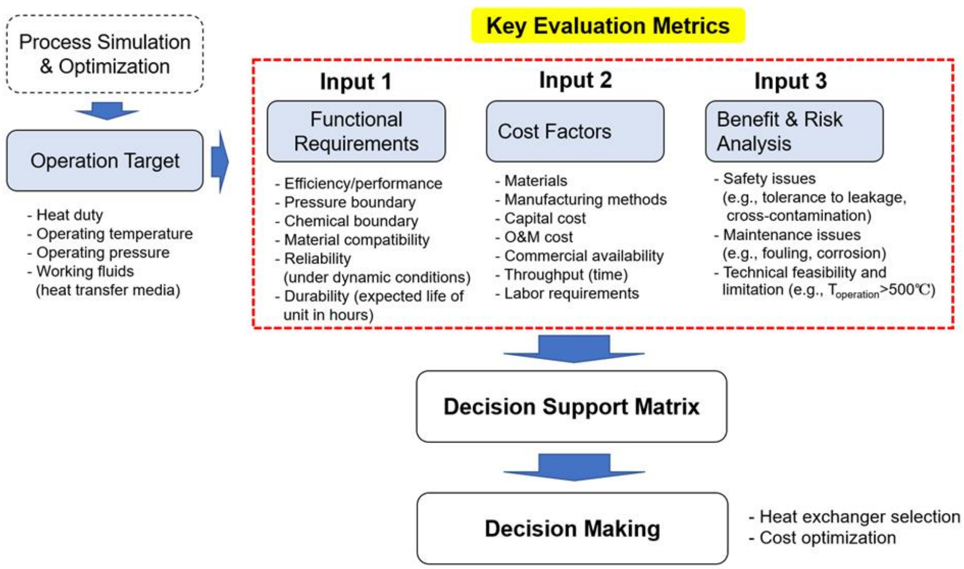


Figure 10. Logical decision path for optimal selection of heat exchanger technology for IES.

Current research focuses on establishing a systematic methodology for strategic, optimal HX selection, where its key components and the preliminary assessment is based on actual application cases. Here, "optimal selection" is defined as selecting a product (i.e., heat exchanger) that best meets various aspects of customer requirements, including technical and economic requirements, based on the detailed technical specifications of the product. Also, the customer indicates the end user of a heat exchanger. The specific demands of the customer (i.e., end user) may differ, including relative importance of each demand or requirement, depending on the particular application of a heat exchanger (i.e., depending on the characteristics of thermal systems to be coupled within an IES). Therefore, it is important to properly take into account the end-user demands, which may vary depending on the application target, in the evaluation process for optimal selection of heat exchanger technology. Considering this, the integrated QFD-AHP method, employed and under study at INL, has several distinct advantages. First, the QFD method allows the evaluation process for heat exchanger selection to consider end-user demands, including both technical and economic aspects, along with the associated HX technical specifications. In other words, the end-user demand and the relevant technical requirements of the HX can be considered together and correlated to make a selection that can best satisfy the customer. Second, the AHP technique can reinforce the quality of evaluation and selection through the QFD process, specifically by providing a robust rationale to prioritize customer demands and compute the individual scores for each candidate heat exchanger with respect to each technical requirement. Third, this approach essentially enables customer-driven decision-making for the heat exchanger selection and provides a consistent way to compare and evaluate heat exchanger technologies regardless of the application target.

Figure 11 shows the hierarchical structure and decision process currently being developed for optimal HX selection and its key components. This indicates that the optimal selection requires multiple steps from high-level to low-level decisions. The first high-level decision is to select the most suitable heat exchanger type for a given application; in the second high-level decision, the critical parts of the selected heat exchanger type, which can best meet both technical and economic requirements, are determined; lastly, a more detailed design optimization, such as design parameters optimization via physical analysis, is performed based on the selection in the first and second levels. Note that the integrated QFD-AHP method, discussed before, is used to make decisions at each level.

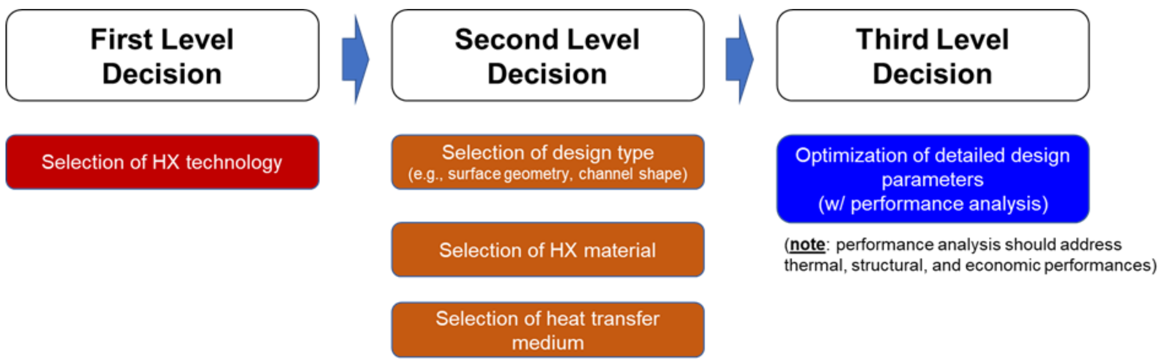


Figure 11. Hierarchical decision path for optimal selection of IES heat exchanger.

Given that the evaluation, comparison, and selection of heat exchanger technologies using the integrated QFD-AHP method essentially requires analysis of the cost factors as well as the technical requirements, such that the associated cost of the selection can also be estimated to some extent.

The IES program seeks to further develop this methodology and, once finalized, apply it to different heat exchanger technologies, such as tube and shell or compact heat exchangers, and also including exotic heat exchanger geometries made by additive manufacturing.

2.3.2 Heat Augmentation

The temperature requirements for coupled processes in an IES might not always line up. For example, an industrial chemical process might need to be run at a higher temperature than a nuclear reactor can deliver. In that case, an option is either to use electricity or gas to augment the temperature to meet the requirements of the industrial process or use a heat pump.

At present, IES program research on heat pumps has been through a Nuclear Energy University Program (NEUP) award [24] with the University of Idaho, which was focused on Chemical Heat Pumps (CHP). CHP are thermochemical energy storage devices with temperature amplification capabilities. Apart from higher energy density, the largest advantage of a CHP system is its ability to improve the quality of thermal energy by boosting delivery temperatures. CHPs feature an energy storage step, an endothermic reaction involving breakage of chemical bonds. Thermal energy is stored as the chemical energy of the products. The energy discharge step is the reverse of this reaction, featuring recombination of the products via an exothermic reaction. By manipulating the reaction conditions, this reverse reaction can achieve higher temperatures than that of the primary energy source driving the energy storage step—thus upgrading the quality of the thermal energy. While this is a promising technology, additional experiments are still needed to demonstrate system robustness for a larger number of dehydration-hydration cycles.

The IES program plans to start doing research into heat augmentation systems. The goal is to establish references of available heat augmentation systems (including thermal and chemical) that can be used in the IES modeling and simulation framework FORCE. This includes thermal requirements, cost, as well as dynamic models that can be used in techno-economic analysis. The developed dynamic models will also be used in the HYBRID framework to assess technical (steady state and transients) feasibility for the coupling of technologies that natively don't have the same temperature requirements.

3 ANALYSIS TOOLS

This section presents the IES program analysis tools used to provide the needed capabilities to model and analyze the various IES cases described. This section is split into three sections: the input data generation needed to start the analysis, the solver capabilities needed to solve the problem, and the output capabilities needed to interpret the data generated and communicate results.

3.1 Input Data

In addition to drawings and technical specifications for the physics models, we also need cost, weather, and market models as inputs for the detailed techno-economic studies.

3.1.1 Advanced Technology Cost Data

To date, IES studies have used cost functions for the various component and system sizes that are generated from a number of sources, including actual quotations from vendors, historical data in literature, and latest publicly available data obtained from APEA-V11 [25]. Cost data (or more specifically "cost functions") development has included the creation of cost trends derived from APEA-V11 data as a function of varying system size. Such data was then used as an input for HERON models for the optimization of IES use cases. For example, in the TES use case studies the resolution of data for the various IES-TES configurations was enhanced by creating a matrix case at different power rates (MW) or energy capacities (MWh).

The most helpful economic drivers for IES cases are the fixed and variable costs and how they scale with changing constructed unit size. Hence, the current data base of cost functions was developed using the following equation:

$$Y = A\left(\frac{D}{D'}\right)^{x}$$

where

Y is the installed cost of the equipment of interest,
A is the reference installed cost for the equipment size of capacity D',
D is the scaled equipment size determined in the optimization or that must be costed,
D' is the reference equipment size that will be fixed and assigned to each piece of equipment, and
x is the exponential scaling factor (<1 implies economy of scale).

In the development of cost functions, *A*, *D'*, and *x* are assigned as constants for each piece of equipment; therefore, the installed cost (*Y*) of the equipment at any scaled size (*D*) can be derived.

When available, actual quotations from vendors and manufacturers were used as an input data to the cost functions. When reliable quotations or solid literature data were not available, the missing cost data were obtained from APEA-V11. Once the costing data were acquired from APEA, the cost functions were developed via the following steps:

1. The equipment and installed costs for all components that appeared in the IES use case models (e.g., turbine, HXs, condensers, pumps, tanks, energy storage material) were acquired to generate a database of cost as a function of equipment size. The installed cost for each piece of equipment includes the

estimate for the following cost elements: equipment and setting, piping, civil, structural steel, instrumentation, electrical, insulation, and paint. Such information are available from APEA.

2. A separate cost function for each component type was created (installed cost as a function of equipment size) using the equation above.
3. When the data resolution (cost as a function of equipment size) from the existing IES use case models was not sufficiently varied to create a regressed cost function for a particular piece of equipment, additional cost datapoints (additional pieces of equipment) were sized, modeled, and added to the database for that particular equipment type. This enhances the accuracy and reliability of the cost functions.
4. In some cases, to enhance the compatibility between the cost data and HERON, the individual equipment cost data (high-resolution data) were used to create major superset models (lower resolution functions) that are compatible with HERON input requirements.
    a. Example: In the TES use case, the individual equipment cost for all the various components (high resolution) were used to create a lower resolution (supersets) that includes the three supersets that are compatible with the HERON codes, namely: (1) charge superset, a group of charge-loop-specific equipment (HXs, pumps, charging streams) with a reference system size (*D'*) that relates to the charging power in MW_{th}; (2) storage superset, a group of storage-loop-specific equipment (hot tank pump, cold tank pump, molten salt, holding tanks) with a reference system size (*D'*) that relates to the storage capacity in MWh_{th}; (3) discharge model, a group of discharge-loop-specific equipment (discharge HXs, additional turbines or capacities, additional condenser or increased condenser capacity, condenser feedwater pump, TES power cycle pump) with a reference system size (D') that relates to the additional electric output from TES during discharge in MWe.
5. A cost function was created for each of the three superset models described above by using the individual cost functions for each piece of equipment falling under that superset model. The cost functions of the three superset models can indicate the additional cost realized of adding TES as a function of system size, which can be used as an input for HERON models for system optimization.

In future work, efforts will also focus on solidifying resources for retrieving accurate costing data for the key components in the IES models and use cases.

3.1.2 Stochastic Input Data

The amount of available data for local marginal prices (LMP), grid demand, and weather phenomena such as wind and solar availability is small, statistically speaking. If each year is taken as an independent sample, most regions only have 15 to 20 years of available data at an hourly resolution, which is a small sample size for statistical resolution, which often requires on the order of thousands of samples.

Synthetic histories are used to introduce additional statistical samples. Ideally, synthetic histories produce yearly data that is physically similar to the available data; that is, it behaves similarly and has the same short- and long-term trends and periodic behaviors. Conceptually, this is like trying to characterize the underlying stochastic process and then sample it for however many realizations are needed to resolve statistical behavior.

The current approach to training synthetic history generators is to model them as a superposition of periodic deterministic behavior and a random process. Fitting selected Fourier modes to the available historical data is intended to capture the deterministic behavior, and Auto-Regressive Moving Average (ARMA) is used to capture the inertial random process [26, 27]. Thus, the deterministic portion is always reproduced by fitting Fourier modes, and the stochastic process generates independent identically distributed samples for unique histories. If an analyst can accurately capture the deterministic and stochastic portions of the physics, then new samples obtained may exceed the bounds of the original training data while still representing physically realistic scenarios. This Fourier plus ARMA approach has been labeled the “FARMA” approach.

There has been some further development of FARMA as assumptions regarding the deterministic and stochastic signals have not held. For instance, the ARMA algorithm assumes that the signal analyzed has variance that is time independent; that is, the general noise of the signal does not vary with varying width in time. This would suggest, for example, that once periodic trends are removed, the uncertainty in how hard the wind is blowing does not vary throughout time. However, we observe that there is seasonality in not just windspeed itself, but the uncertainty of the windspeed. To tackle this, “segmenting” was introduced, which breaks the training signal into windows of arbitrary size before applying the FARMA algorithm. This segmentation allows the signal to be divided into portions in which, presumably, the uncertainty in the detrended signal is consistent.

However, segmenting did not completely solve this issue, as sometimes segment lengths had to be reduced to very small windows, such as 24 consecutive hourly points, before a suitable ARMA could be applied to the detrended signals. Twenty-four time points makes a very small sample size from which to train an autoregressive model, meaning that the quality of this fit will also frequently be poor. This can be observed most clearly with “demand” signals, which frequently show time-dependent variance. For example, the uncertainty in demand during the weekend often shows substantially greater variance than a weekday. This time-dependent variance makes the ARMA a poor model for capturing the inertial uncertainty in practice.

The suitability of a synthetic history generator depends strongly on the application. The IES program uses synthetic profiles of wind, solar, demand, and prices as scenarios on which to test grid energy configurations (or “portfolios”) for economic viability. Thus, the efficacy of the synthetic history generator is determined by how well the synthetic histories represent the various scenarios in which a portfolio may find itself. For instance, if a portfolio is dominated by non-inertial, dispatchable energy sources (that is, sources that can easily ramp production fully between time steps and do not include energy storage), then the continuity of the synthetic signal does not impact the economic viability and instead the distribution of low and high weather and market signals is all that matters. If instead a portfolio has significant non-dispatchable energy sources (such as solar and wind generation) as well as energy storage, the continuity of time and the profile of the demand and prices matters a great deal. In short, the quality of a synthetic history generator depends strongly on the system being analyzed and is difficult to qualify without considering the application.

Although the efficacy of synthetic histories depends on their application, there may be some approaches to provide useful metrics to validate synthetic histories without running the full HERON code. For instance, there are metrics for time series that describe the similarity between the cumulative distribution function of events throughout the signal when compared with the training data. This measure is particularly useful if the target system is largely dispatchable. It is possible that other metrics could be discovered that measure the suitability of the synthetic histories for “high inertia” systems including energy storage or long ramping times between production levels. For these systems, the “jaggedness” or oscillation between high and low values in rapid succession should be similar to the original training data in order to be effective. Research into methods comparing synthetic histories with their training data may yield a suite of metrics that can inform the trainer. By reviewing the suite of metrics, a trainer can understand what behaviors are captured well by the trained synthetic histories, and which are not. An educated decision can then be made concerning which metrics to prioritize based on the application.

Recent efforts in other programs (most notably laboratory LDRDs) have created a modular system whereby more algorithms can be considered for capturing and characterizing both deterministic as well as stochastic components of histories. This opens opportunities for other signal analysis methods, such as long-short term memory, random window decomposition, or wavelet analysis. While these signal characterization tools (and framework) have been developed for other purposes, they could be leveraged for IES analyses. This would also provide opportunity for physics-specific deterministic and/or stochastic process fitting. For example, if the behavior of solar availability is well characterized by a certain stochastic differential equation, the modular approach would allow us to fit historical signals with this physics-driven system and generate new scenarios based on that fitting.

Regardless of whether we use the FARMA process or a more modular *a la carte* process, the sampling of scenarios can be improved. Currently we use an approach that might be described as Monte Carlo sampling, wherein we sample a complex coupled multivariate normal system (coupled in time and across histories) using random sampling and collect samples to determine the overall impact on the economic metrics of interest. While Monte Carlo is a powerful tool for stochastic analysis, it is a rather naïve sampling strategy and can be improved. Monte Carlo samples will always tend naturally to cluster around likely outcomes; however, as shown in the 2016 IES analysis [26], the tails of the scenario distribution tend to drive the economic viability of a portfolio. That is, the unlikely rare events with combinations of low generation with high demand, or alternatively high generation with low demand, affect the economics of a portfolio more than "normal" scenarios, and affect it more than their probability of occurrence would suggest. However, generating these extreme scenarios using Monte Carlo is a computationally costly practice, requiring many thousands of samples to see single samples in highly unlikely regions of the sample space.

For this reason, intentional weighted sampling of extreme events could dramatically reduce the computational complexity of the problem and bring analyses currently outside of the tractable space into practical consideration. If we had a methodology to consider unlikely scenarios that stress a portfolio, but then appropriately weight the economic metrics with the likelihood of the scenario, we could accurately estimate the economic viability of a portfolio with far fewer samples than we currently require. What currently takes thousands of samples may only take a handful, if we can determine which scenarios to sample and how to weight them.

Further, there is a split between intra-scenario sampling and extra-scenario sampling. Determining how to sample a coupled multivariate normal to capture different localized signal behaviors is intra-scenario sampling, in that the sampling all happens within a single synthetic scenario. It is not yet clear how this might translate into extra-scenario sampling, where we intentionally select a subset of scenarios that together, when weighted correctly, allow us to comprehend the economic viability space with far fewer samples. Because the stochastic process signal is added to deterministic process values after sampling, there is no guarantee that a "high" sample in uncertainty space leads to an overall "high" signal after adding deterministic components. To date, efforts have focused entirely on intra-scenario sampling; whether and how this translates to extra-scenario sampling is an important subject for research.

3.2 Modeling Tool Capabilities

This section discusses the capabilities of the FORCE modeling tool suite developed by the IES program to model and analyze IES systems. Individual sub sections for FORCE, HERON, HYBRID, FARM and DRAFT outline the current status of the software and propose future work.

3.2.1 FORCE

The IES program continues to spearhead research, development, and demonstration efforts to produce analytic tools and determine technology candidates, integration techniques, and analysis methods. Because IES increases the number of markets in which energy producers and users can consume or direct energy streams, traditional methods that analyze standalone systems are no longer sufficient. Significant architecture development is required for new tools that can incorporate novel control strategies and balance complex production/demand systems that may include memory and operate within multiple systems' safety limits.

Standard energy planning tools are not well equipped for assessing emerging energy technologies, such as multi-input, multioutput IESs, that will be a necessary part of the solution for net-zero emissions across all sectors of the economy. Many existing tools focus on "single-input, single-output" configurations, such as an electricity generator supporting grid demand. These energy planning tools can also miss cross-sectoral aspects of energy planning, such as a generation resource simultaneously supporting grid demand while also supporting industrial heat users. Hence, the IES team, led by researchers at INL with support from Oak Ridge National Laboratory (ORNL) and ANL, has developed the FORCE ecosystem (see Figure 12). FORCE provides an interface to access several code repositories that individually answer a portion of the problem when evaluating the technical and economic potential of candidate IES. Together, these tools provide the necessary components for portfolio optimization, energy dispatch optimization, process model simulation, economic analysis, stochastic analysis, supervisory control, and workflow automation.

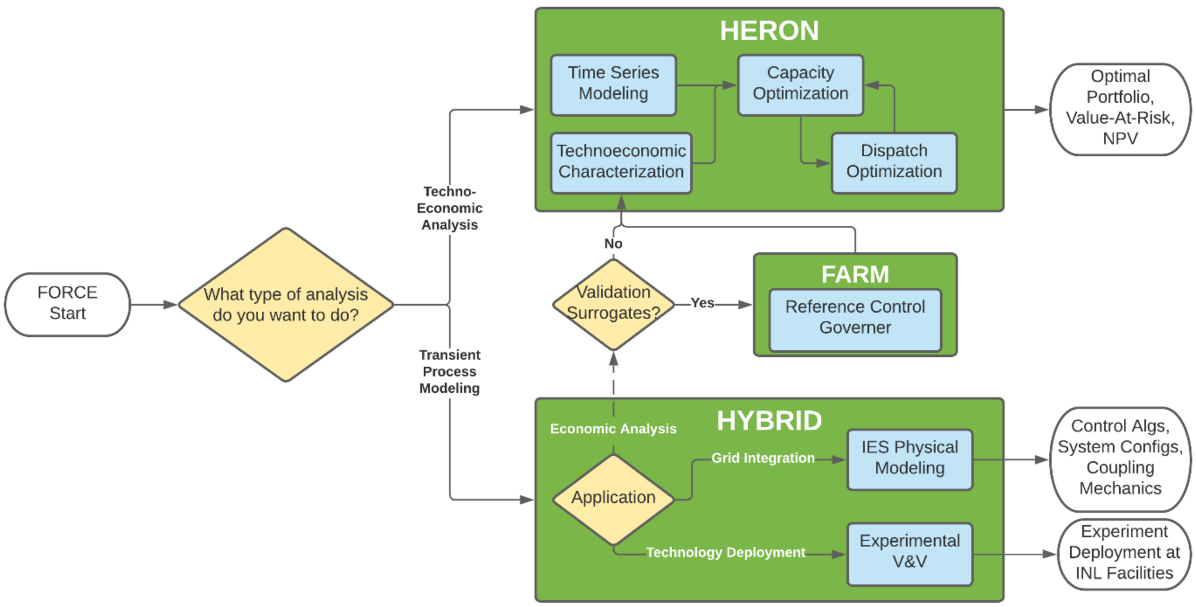


Figure 12. Current FORCE framework.

In its current state, FORCE is a largely conceptual collection of tools that can be divided into two main analysis pathways: long-term (20+ years) techno-economic portfolio planning, and high-resolution dynamic and steady-state process modeling (second by second). Long-term portfolio planning and analyses are performed under FORCE with HERON. High-resolution dynamic and steady-state process modeling analysis is captured under FORCE with the HYBRID repository, where many individual and coupled models are stored for common use. Both HERON and HYBRID make use of several supporting libraries for analysis, including economic metric calculator Tool for Economic AnaLysis (TEAL), stochastic analysis engine RAVEN, and reduced-order modeling resource Feasible Actuator Range Modifier (FARM).

Currently the integration of different FORCE tools is mostly conceptual, i.e., manual and not automated. While results from HYBRID are used to inform HERON analysis and vice versa, to date the interplay has been manual and not formalized. Limited standardization of terms, variable names, and data exists between the long-term planning HERON and transient process analysis in HYBRID. There has been some initial effort in FY22 to standardize pathways for automating communication between tools within FORCE, but additional work is needed.

3.2.1.1 A Typical FORCE Analysis

It is illustrative to consider a typical full techno-economic analysis using FORCE tools. Initially, an analysis case of interest is determined, including the technology coupling of interest, the potential commodity markets, and the desired region of deployment. Once these overarching aspects are determined, then several parallel efforts start, including market analysis, technical analysis, and stochastic systems analysis.

In the market analysis effort, the behavior of commodity markets in the target region are determined. This includes the projected supply and demand of commodities produced by the IES as well as the behavior of these markets. For example, electricity markets are usually based on demand and LMP, which are stochastic in nature and change hour to hour. Hydrogen markets, on the other hand, tend to require stable and consistent supply of hydrogen that remains constant in time. Characterization of all the commodity markets for commodities consumed or produced by the IES enable accurate economic drivers to drive optimal system configurations in a HERON analysis.

In the technical analysis, the technical and economic behaviors of the major components within the target system are considered. Particularly of interest are the technical details surrounding the unit behavior, including production level ramping limitations and transfer functions, which explain how system components consume some resources to produce others. Limits on technical behavior can be regulatory or safety in nature. In addition, the cost and scaling of components in the system need to be determined. This techno-economic analysis of components is performed using tools in HYBRID including Modelica modeling for transient analysis, ASPEN for steady-state analysis, component cost modeling, and literature review to validate all the modeling approaches. The technical and economic characterization of the system components will become the component data in the long-term HERON analysis. During this stage, FARM reduced-order models (ROM) may be trained as physics validators that are higher fidelity than the linear representations in HERON but much faster running than the full transient process models in HYBRID.

The stochastic analysis includes characterizing and training synthetic history generators for the stochastic event data in the target problem. This can include solar and wind availability for markets including significant variable renewable energy (VRE) installation. This also generally includes either stochastic electricity demand or LMP that drives electricity generation. Other stochastic models may also include other fluctuating commodity markets. This stochastic signal training process includes acquiring training signals, selecting characterization parameters such as deterministic detrending and stochastic process lag terms as well as how to subdivide time series into representative clusters and interpolate across years. These trained synthetic history generators should then be validated for use in the target analysis problem.

Once the market, technical, and stochastic analyses have been performed, then the long-term capacity planning analysis can be set up in HERON. This includes adding each component in the system of interest, selecting which components should be optimized for size/scale, and applying stochastic histories. This also includes determining which components have a “fixed” inflexible dispatch and which are dispatchable. The system can then be run in a “debug” mode, which allows the analyst to check nominal dispatch optimization for several synthetic series samples and determine whether the dispatch matches expectations. The debug mode can also be used to check the cash flows in the system and assure all the economic drivers are behaving as expected. Once the user is satisfied, the full HERON run can be started. It is possible that the capacity optimization process may not proceed flawlessly, and some optimization parameters may need to be adjusted for good performance, requiring a few iterative HERON runs to gain confidence in the solutions obtained.

As part of the HERON runs, ROMs produced as part of FARM can be used to validate dispatch optimization decisions. Because HERON only concerns itself with the “manifest” inputs and outputs of each component such as steam consumed and electricity produced, it is unable to track “latent” values such as internal temperature and pressure. FARM provides useful validators to project the manifest values to latent values and check that those latent values are not exceeding determined limits. If there are limit violations, FARM can inform HERON and dispatch optimization will be revisited.

3.2.1.2 The FORCE Future

The process of preparing market, technical, and stochastic analyses before performing long-term economic analysis is complex and requires careful bookkeeping and iteration to assure results obtained are accurate and meaningful. The vision of the FORCE framework is to simplify the complex analysis described above. For instance, analysis of technical models in HYBRID should lead to results that can be read directly into FARM and HERON without manual effort to identify relevant details. Resulting HERON optimized dispatches should be easily imported to HYBRID for performance analysis without manual data manipulation to line up details before running Modelica models. This unification across the FORCE tool suite will lead to streamlined workflows that are less error prone and faster for an analyst to deploy.

The first difficult point in unifying the FORCE toolset is installation. Currently each repository (FORCE, HERON, HYBRID, RAVEN, FARM, and TEAL) needs to be installed separately, and the analyst needs to understand how these codes interact to use them successfully. They each have their own particular installation requirements and process. This presents a significant hurdle to new analysts, especially those that are not comfortable with computer science principles of library interdependence. Ideally, a single-stop installation process should be established that will work seamlessly for most users.

Another point of challenge is allowing analysts to leverage analysis already performed for previous studies. For instance, if stochastic histories are trained on particular projection scenarios for the Electric Reliability Council of Texas (ERCOT) region for one analysis, a future analysis should be able to use those same trained histories if they fit the needs of their analysis. For this purpose, the FORCE repository contains preliminary infrastructure for previous analyses as well as indexing analysis components such as market and stochastic signal characterization. With appropriate documentation on how to build and run analyses, this accelerates future analyses by analysts new to FORCE, by providing examples that can be adjusted to meet the new analysis needs.

Another significant opportunity for improvement in user experience for FORCE is improved output visualization. Existing analysis with FORCE tools has relied on analysts using data from the analysis to generate their own plots and figures. As we understand better what outputs are desired from using FORCE, we can likewise automate the generation of plots and figures that tie together to provide a narrative. While analysts remain free to generate their own plots and figures with the data, some automation of standard figures can save time and effort, and help analysts clearly understand the solutions obtained by using the FORCE tools and provide those solutions to decision-makers with clarity.

3.2.2 HERON

The HERON tool within the FORCE suite was designed to solve the complex problem of stochastic techno-economic optimization of grid energy systems in volatile markets with multiple commodities (see Figure 13). The algorithmic requirement was to solve for the optimal size of components in the system in the presence of uncertainty regarding weather patterns, demand, local marginal pricing for electricity, and other commodity markets. That is, the goal was not to determine the ideal portfolio for one particular energy forecast; rather, the goal was to determine the statistically ideal portfolio given the range of possible futures. This was particularly driven by preliminary analyses [26] that underscored to what extent unlikely high- or low-demand scenarios drove the statistical economics of grid energy systems to a larger extent than median demand scenarios. The impact of loss of load or overbuilding capacity was sufficiently high as to outweigh the low probability of those rare events. Thus, especially for highly stochastic systems, it was determined that it is insufficient to optimize economic metrics for mean scenarios; rather, it is necessary to optimize mean metrics over many potential scenarios when selecting optimal grid energy system portfolios.

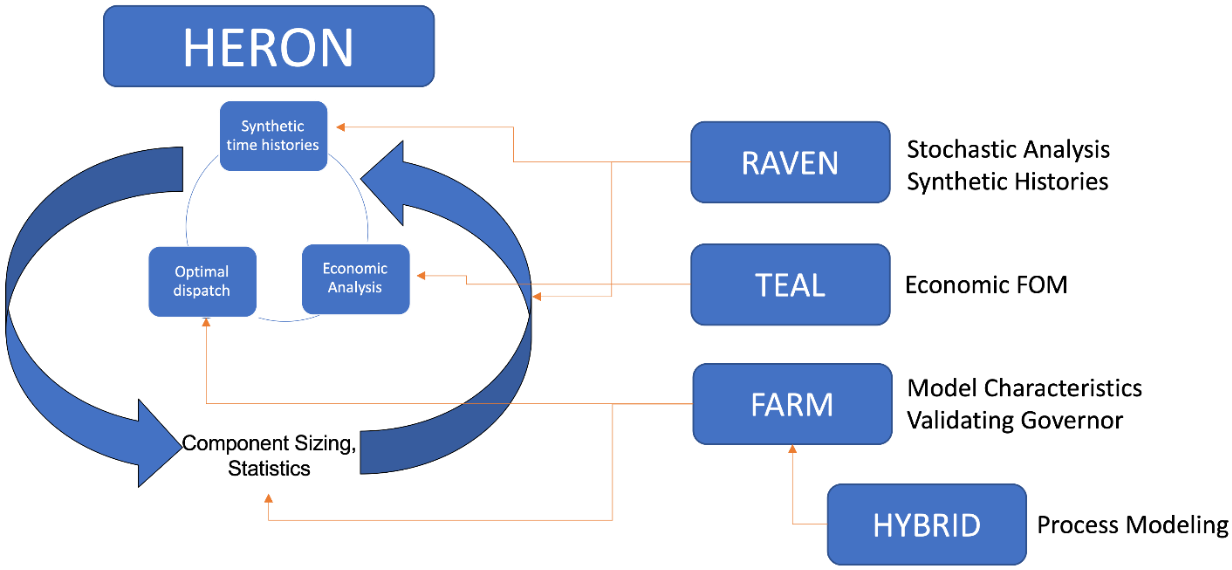


Figure 13. Holistic Energy Resource Optimization Network (HERON).

To solve this multi-level optimization problem, the optimization of capacity was split from the optimization of dispatch. The stochastic analysis tool RAVEN includes tools for so-called "black box" optimization. Black box is a term that refers to the transparency of models. A black box model provides no information about its inner workings, rather only accepting certain inputs and producing certain outputs. A transparent or "white box" model provides details about its operation, usually via algebraic equations or analytic expressions. Optimization of white box models is generally significantly more straightforward than optimization of black box models, as derivatives of outputs with respect to inputs enable optimization algorithms to explore the model response space much more efficiently without heavy sampling.

However, the statistical nature of HERON's target optimization problem does not lend itself to white box approaches. Because the intent is to optimize the portfolio to maximize mean economic metrics, the aggregate performance across many realizations of dispatch scenarios is required, including the dispatch of many models that may not have convenient algebraic form. Thus, portfolio optimization (or capacity optimization) is handled in an outer loop in HERON using black box optimization strategies. This involves heavy sampling of possible scenarios for any chosen portfolio.

For each selection of potential portfolio in the capacity optimization space, it is necessary to determine the expected economic metric value for that portfolio. The expected economic metric has traditionally either been the mean NPV or the value at risk (VAR). Both of these aggregate metrics represent the statistical efficacy of the selected portfolio across the scenarios considered. To calculate the statistical metrics, once a portfolio is selected to consider, many project-length scenarios are generated using stochastic histories such as wind, solar, demand, prices, and so forth. Each set of coupled histories is one "realization" of the uncertain space and may contain 20 to 60 years of contiguous signal data. For each of these scenarios, the dispatch of the components in the system is optimized to minimize costs to meet demand or maximize profitability. The NPV for that scenario is calculated and stored. Once the NPV is calculated for all scenarios, the aggregate metric (usually VAR or mean NPV) is calculated and returned to the outer optimization loop as the metric for the performance of that portfolio. The outer optimizer uses this information to navigate the portfolio space to optimize the portfolio system.

There are some key benefits to this two-level optimization approach. First, the decoupling of capacity and dispatch space allows different strategies to be used at each level. If a custom approach is needed to accurately model and optimize the dispatch for a particular region, that can be implemented independent of the capacity optimization. It also allows the optimization of the capacity to potentially target a separate metric from the dispatch optimization in a bilevel optimization approach, although thus far the target objective has been aligned in analysis cases using HERON. Further, due to the independent nature of the scenarios for dispatch optimization, this problem is highly parallelizable on high performance computing systems. Since each scenario is independent, only one scenario is required to be in memory at one time, which dramatically reduces the resources needed to optimize the full problem.

However, there are some drawbacks to this two-level optimization approach. If a system exists that is entirely algebraic and is sufficiently small that all scenarios and portfolios can be optimized simultaneously, initial indications are that a single level "monolithic" solution may be obtained much more quickly than the two-level black box approach. This is the approach espoused by the Grid Modernization Initiative (GMI) DISPATCHES program, which is developing the software framework DISPATCHES to solve the monolithic optimization problem. Some of the same researchers working on the FORCE toolset have also been working on the DISPATCHES approach, assuring that the same objective is being solved, and the stochastic nature of the system is captured accurately. As such, it is entirely possible that HERON could be positioned to toggle between the two-level RAVEN black box approach and the monolithic DISPATCHES white box approach depending on available computing resources and the nature of the models in use. This would allow the FORCE tool suite to continuously benefit from efforts both by the RAVEN team to improve black box optimization as well as the DISPATCHES team as they improve their monolithic approach.

3.2.3 HYBRID

The HYBRID repository is currently a library of systems models developed in Modelica to characterize the physical responses and interactions of subsystems within IES [28, 29]. Modeling has focused on capturing feedback mechanisms, ramping capabilities, and analyzing control methods within IES that dynamically use nuclear heat. Modelica has been the primary modeling language of choice because of its object-oriented nature that allows for incremental model construction and straightforward component exchange, an FMI/FMU capability allowing use with proprietary models without sharing proprietary data, standardized model connection ports, an inherent dynamic modeling component with a native time derivative, and because the language is flexible to allow for the modeling fidelity to be selected by the user's choices [30]. The HYBRID library models, some top-level seen in Figure 14, are constructed using base components from the Modelica Standard Library and the TRANSFORM library from Oak Ridge National Laboratory [31, 32]. HYBRID modeling allows for system analysis beyond the initial questions of meeting system demands and set-points. Based on HYBRID modeling, the second-level of response to show exactly how those system set-points were met can lead to an evaluation of individual safety, identification of accelerated wear potential, and precise observation of where system demand may be missed in small but possibly important ways.

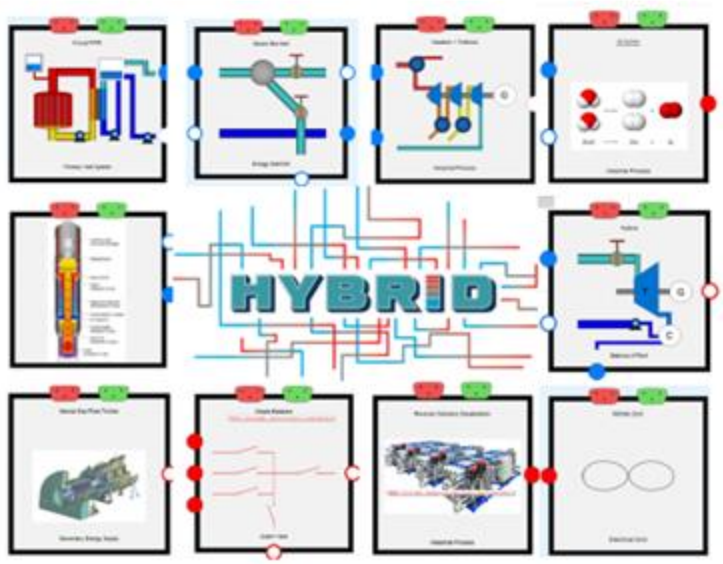


Figure 14. Examples of system simulation level HYBRID models.

The HYBRID repository has been constructed since 2016 and includes a variety of models designed to support analysis of IES for current and future nuclear deployments [33]. Nuclear reactor models now nominally include a current fleet, representative, large-scale pressurized-water reactor; natural circulation and forced flow light-water SMRs; a pebble-bed high-temperature gas reactor with one set up for electricity generation via Rankine cycle and the other via Brayton cycle; and a sodium-fast reactor. Secondary heat generator models include a natural gas fired turbine and a hydrogen-fired turbine. Auxiliary heat product models include water production via desalination (reverse osmosis) and hydrogen production via high-temperature steam electrolysis. Switchyard and electric grid models allow for the electrical interconnection of various subsystems. Multiple levels of balance of plant models have been constructed: single-stage turbine models, dual-stage models with multiple feedwater heating methods, and a stage-by-stage balance of plant model. The energy storage technology library within HYBRID currently includes solid-media sensible heat storage, two-tank liquid sensible heat storage, thermocline liquid storage, phase change materials, compressed air energy storage, liquid air energy storage, and batteries. Experimental models include the TEDS loop and the Microreactor Agile Non-nuclear Experimental Test Bed (MAGNET) loop. The most readily available models are listed in Table 2 below. As Modelica is an object-oriented language, some of the key reusable components are identified. This table is organized via significant IES subsystems and should not be considered exhaustive with regard to all usable modeling components.

Table 2. HYBRID Modelica models presently available.

Modeled Technology	Types of Public Repository Examples	Key Reusable Subcomponents
4-loop general pressurized water reactor	Primary side alone, full IES with HTSE+storage+backup power	LWR core, pressurizer
Light water pressurized small modular reactor	Stand-alone reactor, detailed balance of plant integration, standard balance of plant integration, arbitrage configuration	Natural circulation circuit, pressurizer
High temperature gas reactor (pebble bed)	Rankine balance of plant integration, Brayton cycle direct system, thermal storage arbitrage configuration	Pebble-bed core model
Sodium fast reactor	Stand-alone reactor system	Multi-region core model

Steam manifolds	Full reactor and balance of plant systems thermally connected IES	Dynamically-sized steam ports
Simple balance of plant	Balance of plant for multiple reactor templates	Turbine, condenser
Two-stage turbine balance of plant	Balance of plant for multiple reactor templates, indirectly used in arbitrage configurations	Valves, fluid t-junctions, pumps
Stage-by-stage balance of plant	Based on NRC documents of NuScale design, used in arbitrage IES and for stand-alone reactor operation	Moisture separators, cylindrical coordinate system components
Battery storage	Stand-alone demonstration, FMU demonstrations, IES deployment	Battery
Li-ion battery	Increasing complexity of battery operation examples	3 levels of battery complexity
Sensible heat storage	Stand-alone demonstration, full IES	
Thermocline heat storage	TEDS facility implementation	
Two-tank sensible heat storage	Thermal energy storage use case base model, integrations with LWR SMR and HTGR available	Easily changeable storage media
Concrete solid media	Two configurations, used in energy arbitrage	Easily changeable storage media
Latent heat thermal energy storage	Experiment model	
High temperature steam electrolysis plant	IES demonstration model	SOEC stacks, Hydrogen-steam splitters, Hydrogen-capable turbines
Reverse osmosis plant	Stand-alone demonstrations	RO units, salt-water media packages
Natural gas turbine	Used as electricity backup in IES	Combined gas firing and turbine unit
Hydrogen turbine	Stand-alone example	
Switchyard	Multi-electrical signal example, integrated energy system	
Infinite electrical grid	Used in integrated energy system examples	

The HYBRID library includes a variety of IES configurations based on the currently modeled components. A standard control method is used throughout to facilitate control system exchange. Multiple control systems are constructed for components that can be selected via drop-down menus in the graphical user interface. The IES configurations modeled have supported previous case studies and research efforts.

Some of the models within the HYBRID library have also been built in Aspen HYSYS. These include a variety of industrial process models, reactor models, and balance of plant models. HYSYS is a state-of-the-art steady-state chemical and thermal process modeling platform. HYSYS models are used to determine system sizing and to find steady-state solutions for initialization and verification of set-points within dynamic Modelica models.

The plan for HYBRID is to expand it from a library of transient models to an expansive modeling library usable within FORCE for a variety of applications. The primary tasks to accomplish this include continuing to expand the library of models with new energy applications, construct a library of ROMs, execute validation and verification on the key components, and expand applications by either coupling to safety-type codes or expanding the current modeling library to allow for complete safety analysis.

Expanding the library of models available within HYBRID has multiple goals. New Modelica models are consistently added based on the needs of the IES program, typically through use case requirements. As the IES program continues to support thermal integration of nuclear power, this will lead to an increase in auxiliary heat applications that use combined heat and electricity to drive some form of chemical reaction. Hydrogen production through High Temperature Steam Electrolysis (HTSE) is a starting point for HYBRID and the number of applications should increase with carbon conversion, utilization, capture, and sequestration technologies that will be desired in the future. A second goal of expanding the library of HYBRID models is to create a library of steady-state models that can be matrixed to describe or evaluate the Modelica models that exist. Aspen HYSYS models will likely represent a significant group of these, while other models such as ones created in Matlab, Mathcad, or Python may also fill out the library. By compiling existing models across the IES program and then adding new ones as needed, this should allow users to have a good launching point from which to gather system sizing information and steady-state design information.

ROMs should allow for faster simulation of models developed within Modelica by generating computationally simpler models that can accurately dynamically map the input space of a system to the output space of the system. By training ROMs using the Modelica system models, it should be possible to improve simulation times to support DT integration with hardware in the loop, support techno-economic analyses with simultaneous system simulation, or to do RTO. Efforts are ongoing and will continue to be made to fully understand the methods required to set up ROM generation techniques, nominally using RAVEN, with Dymola or any future integrated development environment. The Dymola-RAVEN interface has been thoroughly tested in recent years and should support this effort. It is desired to construct a library of ROMs similar to the library of steady-state models previously discussed so that users will have direct connections to understand what is being modeled with a given ROM.

Validation and verification are key to assuring model confidence. A variety of V&V methods and levels exist and have been used within HYBRID. HYBRID models are built on first-principle physics: conservation of mass, conservation of momentum, and conservation of energy. To complete the terms of these equations, correlations are used where necessary (e.g., heat transfer and friction loss) and are always sourced from accepted peer-reviewed published research. Building from strong fundamental principles gives credibility to the models before comparison with outside data. Once constructed, there are three more possible levels of V&V that increase in confidence level once completed. The first is face-validation. This method comprises showing results to experts in the field and determining whether results make sense. This method is useful when real-world data is limited, nonexistent, or proprietary in nature. The next step of validation is to compare results with other simulation data that could come from steady-state models, published peer-reviewed research, or from higher-fidelity codes such as computational fluid dynamics simulations. Finally, experimental validation is the highest level of V&V that can be done. Indeed, this workflow has already been established with the TEDS model based on the initial data from the TEDS startup. Validating the TEDS and MAGNET loops is planned in the near term once data becomes available.

Thus far, HYBRID modeling has focused on understanding daily system cycling in a new operational paradigm. System simulation runs are "initialized" at operational states that are or are nearly at steady-state operation and then transients are imposed upon those states to understand system response as the system goes from state A to some state B to either a new state C or potentially cycling back to state A. In the future, this could be expanded in two key areas. The first is to extend simulation to true startup conditions in IES modeling. Doing this requires models to be run much more flexibly, potentially extending valid conditions of present models. Examples of flexibility needs over current models would include adding methods for map-based components (e.g., turbines, pumps, and compressors) to smoothly alter operation from "below" their map location to operate "within" the operating map. Mapped models use setpoints to correlate valid operating conditions within typical operating ranges, the curves within those ranges will go to non-physical setpoints when the system departs the typical operating range. To model outside a typical range, modelers will need to determine physically based methods to transition smoothly from some secondary operating method into the nominal map region. Additionally, there may be a need to adjust flow calculations for low and zero flow conditions which can be computationally very expensive as denominator terms approach zero. The second main expansion area proposed is safety analysis. There are multiple potential pathways in this space. The first is to expand HYBRID to include additional modeling tools and languages to cast current Modelica models into codes such as RELAP5-3D to allow currently existing safety codes conduct the analysis via identical model construction. A separate pathway would be to introduce sufficiently high fidelity to perform a safety analysis within Modelica models themselves. This may require increasing the fidelity level within certain components and would depend on model V&V. An intriguing extension of safety analysis within Modelica would be allowing for component failure, extending some work already being done within IES, and allowing those changes to propagate through systems models. Components would need to have some form of logical physical operating mode triggered by numerical events within simulations.

3.2.4 FARM

FARM supports the HERON plug-in to solve the power dispatch problem. The solution obtained represents the optimal dispatch meeting the limits on production variables and the corresponding rates of variation (explicit constraints) as well as the limits on the process variables tied to the service life of equipment (implicit constraints). Given the challenge of the computational burden and the need to address it, the optimization problem is decomposed into a two-stage process. First, the HERON power dispatcher estimates a solution that meets explicit constraints on ramp rates. This solution is a first estimate and does not necessarily meet implicit constraints, given HERON's partial characterization of the system dynamics ("low-resolution physics"). Second, FARM refines this solution by using the results of the HYBRID high-fidelity model to capture the system dynamics ("high-resolution physics") and enforce implicit constraints (Figure 15). The initial version of the code (FARM-Alpha) was released by ANL in January 2021 [35]. It was followed by FARM-Beta [36] (January 2022), FARM-Gamma [37] (April 2022), and FARM-Delta [38] (July 2022). In Figure 16, the FARM-Delta scheme is represented.

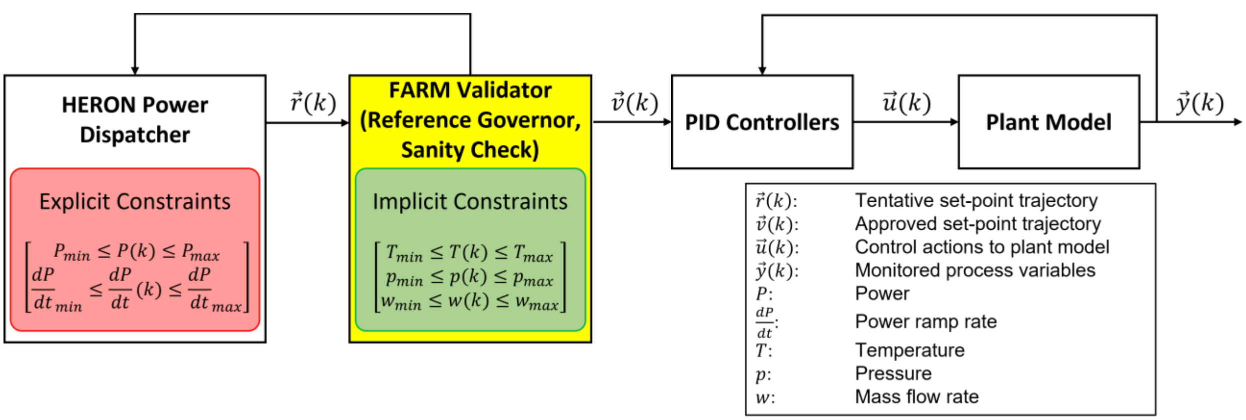


Figure 15. Power dispatch scheme addressing both explicit and implicit constraints.

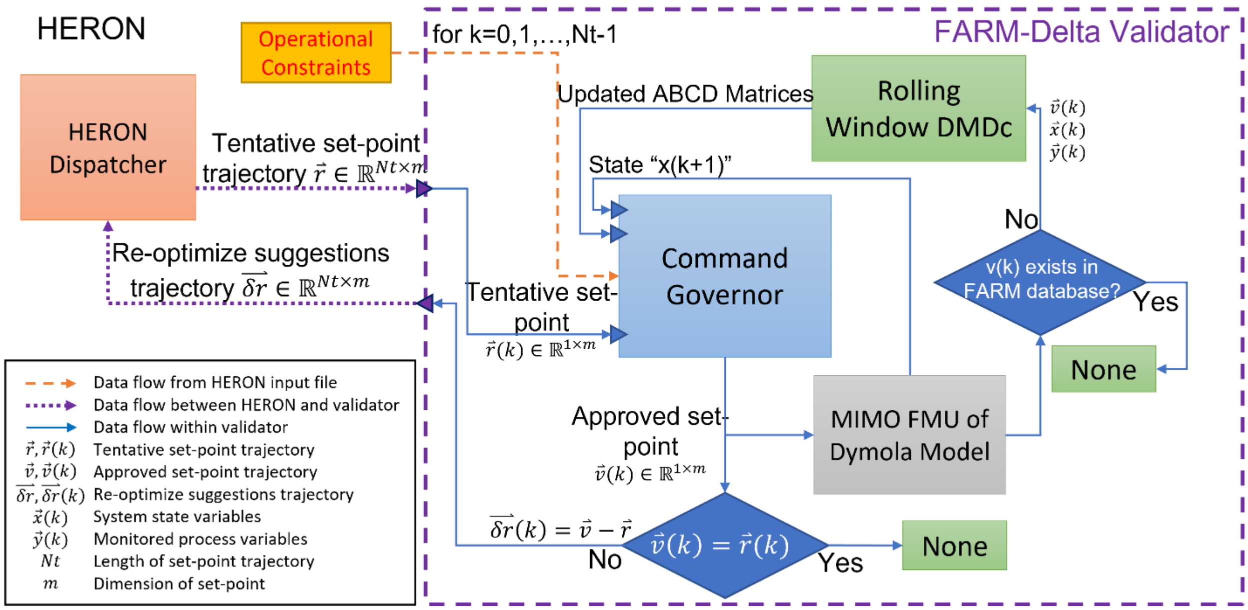


Figure 16. Graphical representation of the optimization scheme implementing the latest FARM-Delta validator (FMU coupling).

FARM's Support of ROM and High-fidelity Downstream Models

As shown in Figure 12, FARM serves as a bridge between the HERON and HYBRID modules. FARM derives ROMs to support the former to evaluate the optimal dispatch and adopts the high-fidelity model simulations provided by the latter to refine the tentative solution. In its bridging role, FARM is capable of handling both ROMs and high-fidelity models for power dispatch optimization purposes.

As for ROM, FARM is capable of both deriving and using ROMs. In the latest releases (FARM-Gamma and FARM-Delta), FARM handles ROMs in a two-stage process. First, FARM derives ROMs during the "Self-learning" stage, where the ROMs are derived from HYBRID simulation through a data-driven method (Rolling Window Dynamic Mode Decomposition with Control [DMDc]). These ROMs can be indexed by the scheduling parameter (e.g., the power level) to capture the system dynamics under various operational conditions. Second, FARM uses the ROMs in the "Dispatching" stage to predict the system response corresponding to the optimized power transients without compromising the efficiency and the safety of the system.

As for the high-fidelity models, FARM can use them in the form of FMUs to further validate the optimized power set-points and improve the knowledge of system dynamics. When simulating FMUs in the Python environment, FARM does not handle the FMUs as a black box (i.e., imposing input and gather output) but has access to all the available process variables. Thus, FARM can (1) maintain a record of the response of the process variables of interest, (2) select the state variables and derive ROMs, (3) validate the tentative set-points on-the-fly, and (4) provide numerical feedbacks to the HERON dispatcher. Currently, Dymola-derived Single-Input-Multiple-Output and Multiple-Input-Multiple-Output FMUs are supported by FARM, and the interface can be easily adapted to other high-fidelity models.

FARM's Core Algorithms

The different releases of FARM either use the scalar reference governor (RG) or the vector command governor (CG) [40] for constraint enforcement. Both of the algorithms evaluate the maximum output admissible set (MOAS) (i.e., a set of linear inequalities constructed by using the state-space matrices, the prediction time horizon, the current system state, and the operational constraints). This set can be represented as a multi-dimensional admissible region for the power set-points (i.e., the power set-points laying inside the MOAS will not lead the system to violate the operational constraints within the prediction time horizon). However, different releases of the FARM software utilize the MOAS differently.

In FARM-Alpha, Beta, and Gamma, the scalar RG method addresses single-input systems only. The RG reads MOAS line-by-line and linearly scales the tentative set-point into a value permitted by the MOAS, thus ensuring the operational constraints are not violated.

In FARM-Delta, a vector CG method addresses multiple-input systems. The CG constructs an admissible region as a N-dimensional polytope defined from MOAS and performs a quadratic optimization to find a solution vector that minimizes the geometrical distance to the tentative set-point vector, as shown in Figure 17. FARM-Delta will be the foundation of all the future developments and applications. The capability of performing multi-input online system identification, visualizing the admissible region and performing the quadratic optimization will be further deployed.

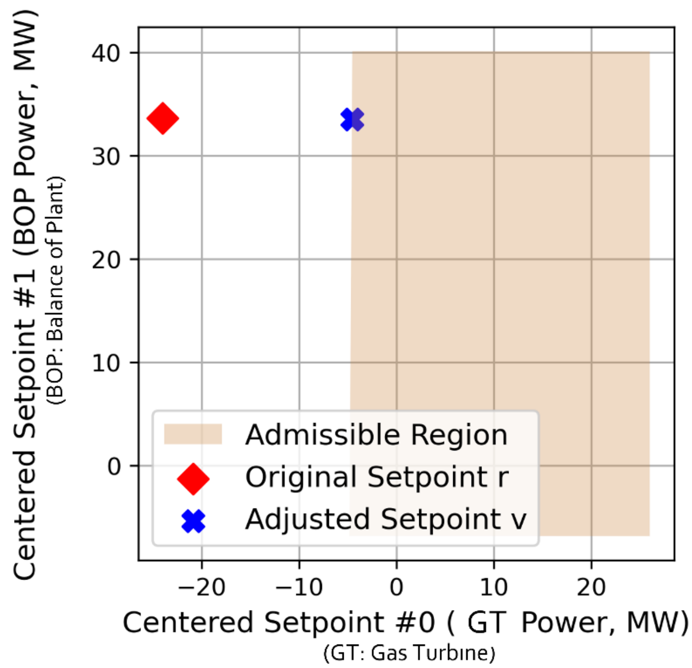


Figure 17. Admissible region and set-points optimization for a two-input system in FARM-Delta.

FARM's Next Step: Provide Help to RTO

The automated procedure for selecting the state variable will help in deriving time-variant ROMs for the RG/CG algorithm, starting from the simulation outcomes of a high-fidelity model. At the same time, there are other valuable applications of this capability (i.e., FARM might support RTO) [41] to solve the power dispatch problem over short time-horizons). In the power dispatch problem [38], the optimal solution is calculated for 12 hours using constant price, constant cost, and pre-defined market demand. In RTO scenarios, prices, costs, and demands are continuously updated, and decisions are expected to be made with short notice (a few minutes ahead) based on the real-time conditions of IES components. The latest FARM-Delta nearly provides a seamless solution. Thanks to the FMU-based wrapper, other high-fidelity models can be simulated, and the system state can be retrieved by tracking the response of candidate process variables. The DMDc can then track the evolution of these variables during the optimization process to derive the ROM of the whole IES unit. As shown in Figure 18, FARM can provide assistance to RTO due to two unique capabilities: self-learning and optimization.

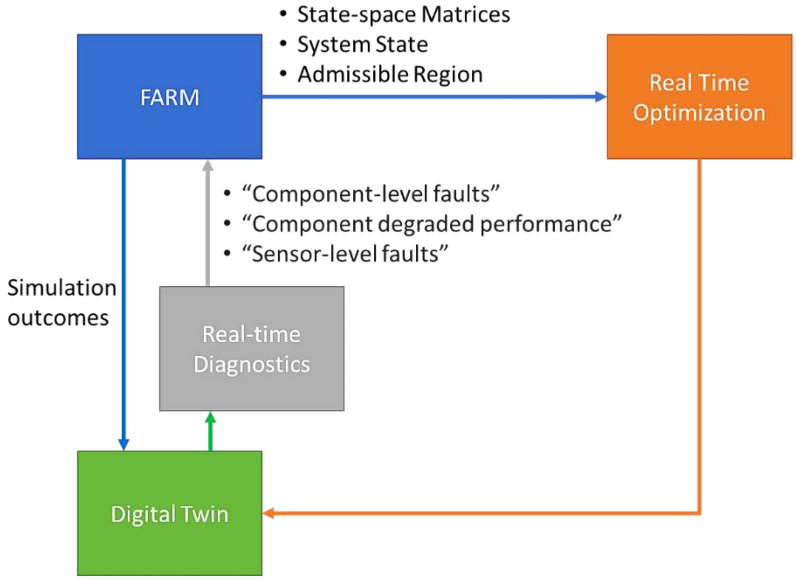


Figure 18. FARM's capabilities that can help RTO.

First, FARM's unique self-learning capabilities could help RTO in identifying the optimal set of state variables and deriving a suitable model representing its dynamics. FARM can select the set of state variables to monitor system state (this feature is under development). This task will be done by an algorithm called Dynamic Mode Decomposition Control with Recursive Feature Elimination (DMDc-RFE). In addition, FARM can track the evolution of state variables and derive state-space representation matrices that can favor the adoption of advanced control schemes (e.g., Model-based Predictive Control [MPC]). In addition, this system identification algorithm can be activated during the simulation of the power dispatch, so that faults/degraded operating conditions can be suitably addressed.

Second, the FARM optimization capability can support RTO to solve the power dispatch problem over short time-horizons. FARM returns optimal value and admissible region of set-points and other key process variables, and FARM's core algorithm (RG and CG) constitutes a supervisory control layer on top of proportional–integral–derivative (PID) controllers.

These capabilities enable FARM to support operation of an experimental facility (e.g., TEDS [8]). In this case, the data to derive the matrices would come from sensor readings. To ensure a trustworthy data flow in case of sensor-level or component-level faults, a "Real-time Diagnostics" module needs to be coupled to the DT and FARM (Figure 18).

FARM's Future Application: Reduce Human-Factor Related Mistakes Through Visualization

As mentioned above, FARM-Delta has human factors applicability given its ability to estimate an admissible region as a N-dimensional polytope defined by MOAS. When cast visually this can serve as a valuable operator aid for understanding in advance the system process variable response for a planned transient. As shown in Figure 19, the response of three process variables during a planned transient is plotted as three-dimensional scatters together with the tetrahedron-shaped admissible region, and the scatters outside the admissible region are marked as red pentagrams. In this way, constraint violations would be promptly detected, thus helping the operator to evaluate the feasibility of the scheduled transients. Alternate visualizations such as spider diagrams are also viable candidates.

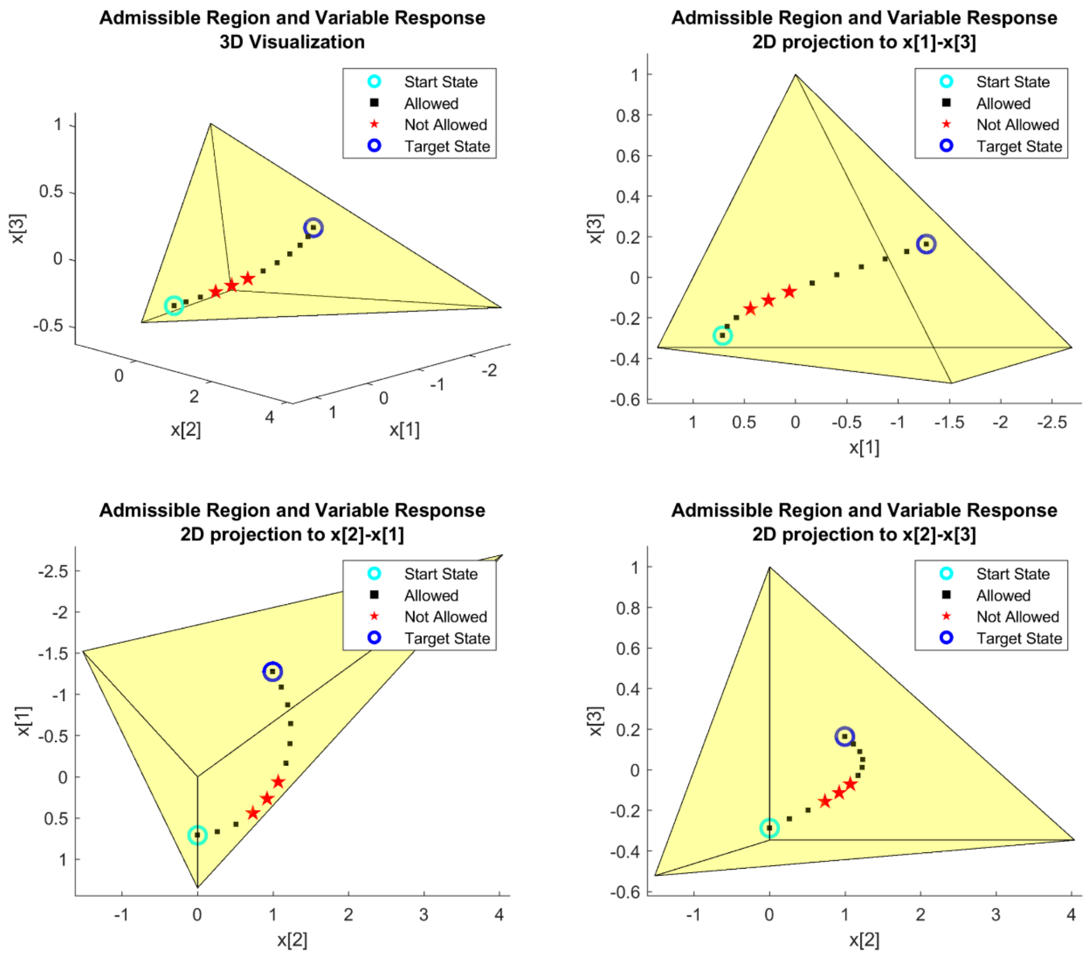


Figure 19. Admissible region and variable response in planned transient.

The N-dimensional envelope cannot be directly used by operators (for N>3 scenarios, it cannot be visualized). A feature selection to down select a maximum of three process variables to be visualized must be performed (especially the variables describing crosstalk between components).

3.2.5 Dynamic Reliability Analysis Framework and Toolbox (DRAFT)

The reliability framework developed at ORNL aims to ensure that IES's components and systems operate reliably. The framework (1) gathers component and system operational data from HYBRID, the IES simulator, using the Transient Simulation Framework of Reconfigurable Modules (TRANSFORM) models, (2) builds relevant probabilistic models, and (3) estimates the failure rates to forecast the lifetimes of the selected IES aging components and systems. The framework RAVEN plug-in provides predictions of reliability-related costs (e.g., planned and unplanned maintenance costs) for the overall stochastic cost optimizer, HERON, along the time horizon under consideration (e.g., a day, a week, or two weeks) or for the reactor operational life (~60 years) for selected components and systems. The reliability framework plug-in for RAVEN (DRAFT) will be open sourced.

The reliability modeling framework DRAFT consists of two submodules, as detailed below.

1. Accelerated Aging Module: This submodule is designed to take simulated Dymola operational data for component level assessment and calculate *ß* and η values, estimate failure rate of the component, optimum maintenance interval along with generating cumulative distribution

functions (CDFs), hazard rate, and Weibull plots for the data.

Inputs: HYBRID component simulation (number of samples, failure/suspension cycle counts)
Outputs: Estimated η, scale, and ß, shape parameter, for Weibull fit, reliability, and hazard rate functions

2. System Reliability Module: Stochastic Petri Nets model is used to capture system interdependencies and system failure rates of the IES.

   Inputs: Accelerated aging module failure estimates based on component simulation
   Outputs: Mean wait time at a state, transition probabilities

The Accelerated Aging Module uses the maximum likelihood estimation method; the likelihood function is formulated, and suspended data are solved for considering Weibull as the underlying lifetime distribution. The ß and η parameters are used in reliability equations to determine the life-cycle qualities of data sets. The corresponding probability density function, **pdf**, is given by:

$$f(t|\beta,\eta) = \frac{\beta}{\eta^{\beta}} t^{(\beta-1)}\, exp\left\{-\left(\frac{t}{\eta}\right)^{\beta}\right\}, \text{for } \eta > 0, \text{and } \beta > 0. \quad (1)$$

In addition to the shape and scale parameters of the fit Weibull distribution, the Accelerated Aging Module can produce two plots, as shown in Figure 20 and Figure 21. Figure 20 depicts how well the Weibull distribution fits the failure data using probability paper, and Figure 21 is a plot of the fit Weibull cumulative distribution function and its corresponding confidence bounds. A probability paper or probability plot is a graphical methodology for assessing the fit of a probability distribution (e.g., in this case, the Weibull distribution) to a data set. In this type of plot, the horizontal axis is the lifetime or the value of the random variable and the vertical axes represents the CDF of the data. A straight line is fit through this data using linear regression and departures from this straight line indicate deviations from the specified distribution. Thus, an adequate fit Weibull distribution with ß and η parameters will be exhibited by the data points aligning well with the best-fit straight line.

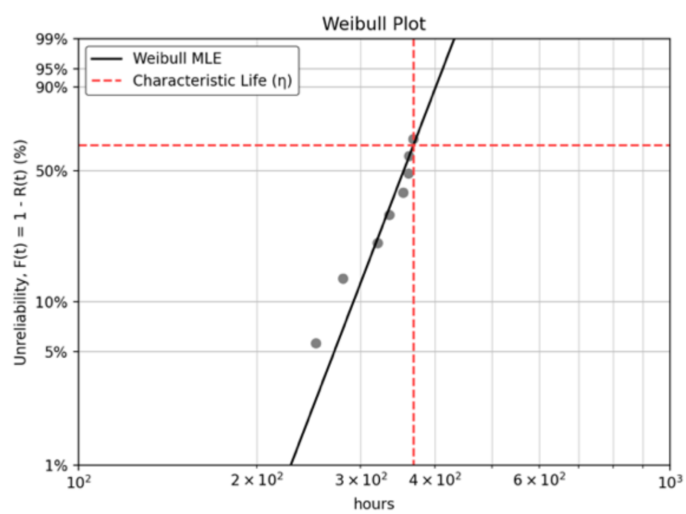


Figure 20. Weibull probability paper plot for sample failure data.

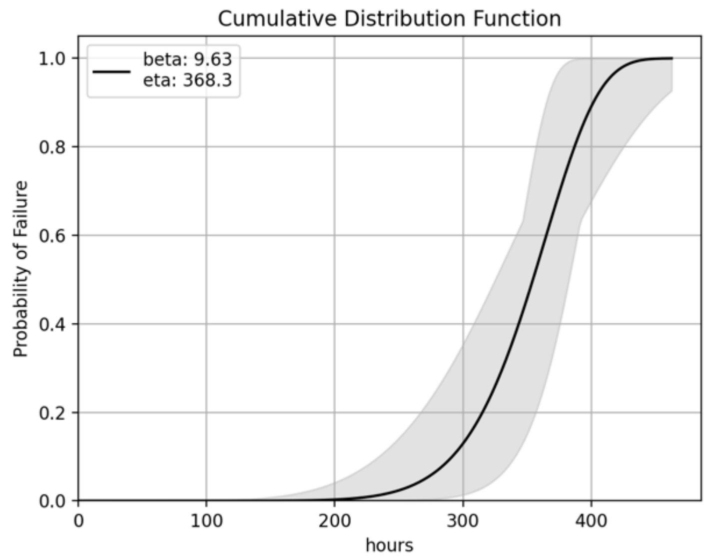


Figure 21. Weibull cumulative distribution function fit to the sample data.

The DRAFT reliability code developed at ORNL will be integrated in the FORCE tool suite. The final product will include the following items:

- A code module consisting of two submodules: The Accelerated Aging and System Reliability submodules.
- User's guide
- The reliability/FORCE integration will cover the functionality to add reliability driven cash-flows to FORCE TEAs (coupling to TEAL)
- Additional functionality of the reliability module—informing asset operation (i.e., coupling to FARM as well as cybersecurity functionalities [coupling to HYBRID])—will be coupled to FORCE later (thermomechanical constraints for the individual subsystems and components)
- Digital Reliability Twin of a Facility for IES Exploration (e.g., Facility to Alleviate Salt Technology Risks (FASTR)).

The reliability framework plug-in for RAVEN will be open sourced using a dynamic reliability method to compute the probabilities of occurrence of the various conditions with respect to time. Since IES demand and dispatch change throughout the optimization phase, the repair/replacement plans and intersystem dependency of systems dictate coupling the reliability model with FORCE.

3.2.6 Resilience

The IES program currently does not include the value of resilience in analyses. This section describes a new, future application for FORCE.

There are many potential benefits to coupling NPP in IES configurations. Two of the main considerations are the flexibility that leads to benefitting from arbitrage as well as the potential revenue stream of providing heat for generation of secondary commodities to markets that nuclear power has not traditionally supported.

Another possible benefit of nuclear IES systems is improved resilience. In this context, by resilience we mean the ability of a system to respond to sudden changes in boundary conditions, particularly sudden changes in energy demand. These changes could either be unexpected increases or decreases in demand.

Resilience metrics measure the ability of a system to quickly respond to these sudden changes. Resilience has benefit to existing energy systems that experience increased volatility due to non-dispatchable VRE systems and limits to existing response mechanisms due to economic or policy pressures to reduce or eliminate carbon emissions.

While the market for added resilience is small and shallow in existing energy markets in the United States, decreased resilience from VREs and expensive or limited use of responsive carbon-based generators may cause modern energy markets to rethink the benefit of resilience in their grid systems. FORCE tools can approach resilience as an optimization consideration in portfolios in several possible pathways. The most direct path would be to quantify expected market valuation of added grid resilience and let this economic opportunity drive selection of technologies within a portfolio optimization. Alternatively, resilience could be considered a separate optimization parameter, which would result in a weighting balance between profitability and resilience in optimization, creating Pareto fronts of solutions with a mix of resilience and profitability. Finally, resilience might be considered a boundary condition, requiring a certain amount of grid responsiveness that constrains optimal profitability. Regardless of the approach, determining and implementing methods for HYBRID to be used to quantify resilience in a system would enable more informed optimization options in HERON and give another tool to measure system effectiveness.

3.2.7 Market Interactions and Capacity Expansion

The FORCE tool suite currently does not include a capacity expansion model. Instead of developing its own model, the IES program is planning to couple an existing, suitable, and expandable model. This section describes capabilities that a future coupled capacity expansion mode should include.

Market Dynamics and Technology Adoption

One dimension on which the FORCE framework should develop is with respect to its treatment of market dynamics. Many of the problems where FORCE is applied represent technologies that could be game changers for how markets work. For example, an IES makes possible energy arbitrage (i.e., storing energy during periods of low prices and selling stored energy during periods of high prices). Current modeling reflects a "price taker" assumption. This means that the modeling framework takes energy prices as given, and the arbitrage decision is based on observed energy prices. The problem with this approach is that if energy arbitrage is good for one type of agent in the marketplace, then it is probably good for many agents. And if it is good for many agents, all of whom engage in energy arbitrage, prices consistent with a price-taker assumption are no longer valid. The combined effect of the agents impacts price formation, and that is not currently reflected in the modeling framework. Dynamic price formation could be developed into the FORCE framework in many ways, two of which are computable general equilibrium (CGE) modeling and the Bass diffusion approach to technology adoption. CGE modeling is based on elasticities of supply and demand and the cross partial elasticities for specified sectors of the economy. The elasticity information shows how a shock (like technology innovation) in one sector of the economy impacts other sectors of the economy. Bass diffusion models the rate of technology adoption based on agents who choose to innovate (early adopters) versus those who choose to imitate (those who want to see technology demonstrated by others, first). Either of these, or possibly other ways, could lead to endogenous price formation instead of the constraining, price-taker approach.

Bayesian-updated Cost Forecasting

A point related to that of market dynamics mentioned above is Bayesian-updated, cost forecasting. In the example above, market evolution brings with it price formation based on the number of agents in a market deploying technology. If this turns out to be the case, then cost will need to evolve commensurately. As more and more entities adopt technology two forces will drive costs down: learning curve effects and economies of scale and scope. That is, as the stock of knowledge about a technology concept builds then it will be disseminated across the industry (i.e., learning) so that costs across the industry fall. But it will also be the case that early adopters will give way to industry scale up, which means that because of economies of scale, then unit production costs will fall. So, cost updating consistent with assumptions on market deployment is one aspect of dynamically updating cost. Related to this need is that of uncertainty ranges on costs. FORCE represents stochastic processes in energy prices but not as much detail is currently provided for technology costs. In addition to updating technology costs commensurate with industry to decrease uncertainty, one should also consider incorporating uncertainty ranges.

Market Model Validation

The accuracy of FORCE must be demonstrated. Model validation is an area where FORCE should be tested. A case study, like the use cases where FORCE is applied today, could be constructed to evaluate a known, established technology as it emerged for a stake in the market. Then the results of the use case could be compared with historical data. For example, suppose FORCE is used to evaluate the build-out of solar technology in an energy system. Data can be obtained to characterize exactly how solar became established in the market. Similarly, a use case could be developed reflective of, for example, the year 1980. If FORCE was applied to 1980 input data, how well would it replicate the historical build-out of solar? An exercise such as this would do much to define gaps in the FORCE framework, as well as demonstrate its strengths.

Theoretical Model of IES

It is important to understand the perspective FORCE represents—a utility owner, a grid operator, a merchant generator, or other? To better understand this, developing a theoretical model could help. Suppose a utility owner calls upon the FORCE framework to model an investment decision, but the owner has a portfolio of electricity generators in addition to the investment under consideration. Alternatively, the generator may suspect that a competitor engages in strategic interactions. A theoretical model would help to articulate the owner's problem and guide the application of FORCE such that it is suited to the situation. The complexity of the problems in the IES space suggests that it is not likely that a closed form, analytical solution to an optimization problem will be attained; hence, the theoretical model would point to the need for numerical solution. However, the theoretical model would be useful for ensuring that all the relevant components of the problem are represented.

3.3 Visualization, Outputs, and Result Communication

Until recently, almost all the analysis using FORCE tools was either performed by developers of the tool or by teams including the tool developers. This is to be expected for tools that are newly developed. As the FORCE tools mature, however, improvements both to the user interface and output feedback are necessary. Tool developers have traditionally been comfortable with text-based inputs and command line code operation, as well as postprocessing their own data to generate plots. Many analysts, however, are not comfortable with these interfaces and would benefit from some automation of both inputs and outputs. On the input side, graphical user interfaces (GUIs) have become standard in much of computational analysis. While it is costly to maintain a fully functioning GUI while tools are undergoing significant development, as the tools begin to stabilize in terms of inputs and outputs, it becomes more practical to design and maintain a GUI. Some recent efforts have demonstrated dynamic GUI that are rebuilt based on input changes; however, this circumvents the main purpose of the GUI, which is to provide a guided experience in completing analysis. Experience has shown that the more dynamic adjustments to input are made for a GUI automatically, the further it strays from a streamlined, guided analysis experience.

The roadmap currently envisaged for input processing is a tiered approach. Three tiers are planned for:

- **Enhanced Integrated Development Environment (IDE)** for input processing: while enhanced IDEs are still text editors, they allow the use of widgets that can graphically enhance and guide input creation. This allows to cater to users with widely different levels of expertise of using the code. In particular, new users can be guided with templates and wizards, while expert users of the code can still access all the details of the code.

  One area where an enhanced IDE can significantly help is for the building of synthetic data ROMs. Currently, ROMs that are needed as inputs for FORCE analyses are trained and built outside of

FORCE. That includes ROMs for electricity market price data as well as ROMs for weather data such as wind or solar availability. The enhanced IDE should allow creation of synthetic history ROMs as part of the FORCE workflow. Key elements that are needed include (1) easy raw data visualization, (2) easy selection and visualization of detrending methodologies and effect on the raw data, and (3) visualization of white noise in the data. These key elements all contain subsequent smaller elements that need easy visualizations as well, such as effects of data clustering and time slicing.

Once input data has been visualized and pre-processed, the enhanced IDE will offer an easy way to select and pre-fill template work flows depending on the type of analysis the user is looking for. As mentioned, beginner users will be offered a wizard that walks the user step-by-step through input creation while expert users will benefit from the IDE's enhanced text manipulation capabilities.

- **Webtool**: The next step is creating a webtool that is able to promote the functionalities of the software in an easily accessible environment. The goal of the webtool is not to offer the full suite of options of the software, but rather have some precomputed examples under the hood which users can easily access and study to understand what the capabilities of the FORCE suite are. The webtool will include sliders and radio-buttons for some of the most interesting input parameters, like cost or price forecasting modes. Users can change these inputs and will immediately see the effects on the output variables plotted on the website (e.g., economic figures of merit).
- **Commercial GUI**: The last tier is a commercial GUI. Currently, private industry is working on commercializing the FORCE tools, which includes a GUI offering a broad spectrum of capabilities.

On the output visualization side, standard plots need to be created to effectively communicate results to different audiences. The metrics to communicate will be defined by working with communications specialists. A standard way to communicate also allows one to build recognition (branding) of the FORCE tool suite.

4 SUMMARY AND TIMELINE

Since inception of the DOE-NE IES program, several program and modeling visions and roadmaps have been published. In 2017, the last modeling and simulation capability development plan was published. In 2020, a comprehensive roadmap for the DOE-NE IES program was published. The current report is meant to update the 2017 modeling and simulation capability roadmap and complement the IES overall program roadmap published in 2020.

As mentioned, modeling and simulation has a support function in the IES program. Software capabilities are driven by "use cases." Industry and government priorities drive the selection of use cases and associated technical and economic questions. The selection of which use case to tackle next is driven by the overall program and technology deployment roadmap. However, modeling and simulation offers to develop a methodology including a set of metrics that will help to rank possible future use cases. Metrics include economics, overall energy efficiency, GHG emissions avoided, social justice, and more. With such a methodology, the IES program will be able to validate and inform expert opinions on the ranking of future use cases.

Table 3 shows the timetable for modeling and simulation analysis for current and upcoming use cases. As previously described, analysis of use cases includes the identification of thermal and electrical requirements as well as cost for construction and operation. With this data, technical and economic feasibilities of a particular IES configuration are investigated.

Table 3. Roadmap for use case analysis.

	FY22	FY23	FY24	FY25	FY26
Synfuels					
TES					
Carbon Convertion					
Ammonia					
Metrics developed					
New Use Case (1)					
New Use Case (2)					

In addition to continuing to analyze use cases, the development of physical dynamic models, needed inputs, and FORCE tools capability enhancements is also continuing within the IES program. Figure 22 shows the proposed future FORCE framework that include ORCA (Optimization of Real-time Capacity Allocation) for RTO, DRAFT for reliability tracking as well as a capacity expansion module. Table 4 shows a timeline for the different pieces of software and models that need to be developed. Note that FORCE includes the dynamic model library HYBRID. Expansion of HYBRID aligns with the models needed to support use cases (i.e., as long as there are use case analyses), HYBRID is still under development. Development of a GUI is targeted for completion in FY24.

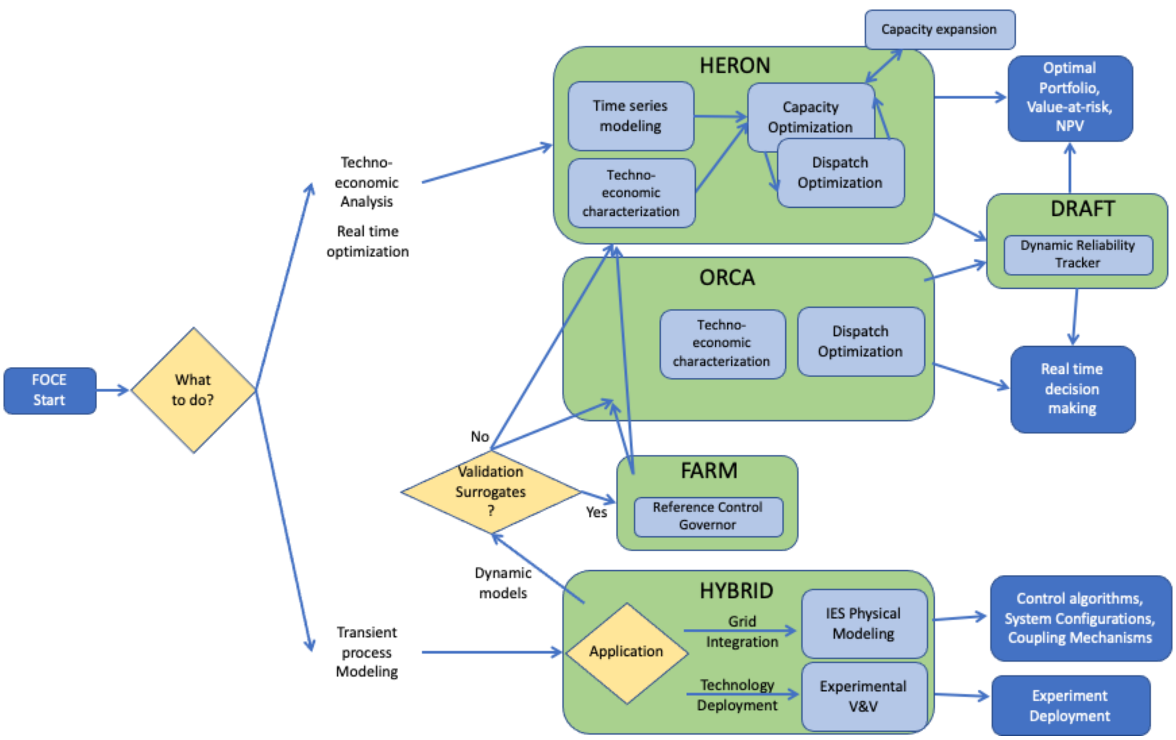
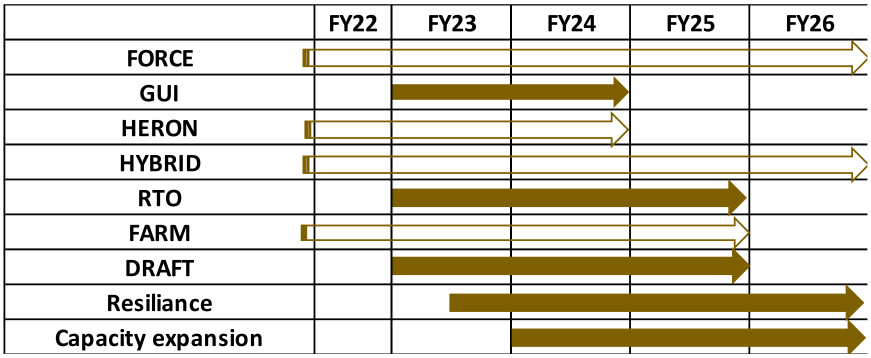


Figure 22. Proposed future FORCE framework.

Table 4. Roadmap for FORCE tool development.



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