INL/RPT-23-03146
Revision 0

HYBRID Modeling Validation and Verification Status Matrix

February 2023

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Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

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ABSTRACT

The HYBRID modeling repository is a premier resource for integrated energy systems modeling. HYBRID models have been developed since 2015 to describe the physical operation of tightly coupled thermal systems including power generators, thermal transport systems, thermal storage, thermal-to-electric conversion systems, and other thermal applications. Due to the increased size of the repository, a concise summary matrix of available models is needed. This matrix will consolidate not only the list of available models but also indicate original information sources, publications with model examples, and levels of validation and verification that exist for the models. Validation and verification (V&V) levels begin with simplified algebraic relationship and advance to dynamic data validation. Moving forward, as new models are contributed to HYBRID, their V&V levels will be included, updating this matrix through annual reports.

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LIST OF ACRONYMS

BOP	balance of plant
CFD	computational fluid dynamics
CTES	concrete thermal energy storage
DMDc	dynamic mode decomposition with control
HTGR	high temperature gas reactor
HTSE	high temperature steam electrolysis
IES	integrated energy systems
INL	Idaho National Laboratory
IPWR	integral pressurized water reactor
MAGNET	Microreactor Agile Non-nuclear Experimental Test Bed
ODE	ordinary differential equations
PWR	pressurized water reactor
RAVEN	Risk-Analysis Virtual Environment
ROM	reduced order model
SFR	sodium fast reactor
TEDS	thermal energy distribution system
TES	thermal energy storage
V&V	validation and verification

HYBRID Modeling Validation and Verification Status Matrix

1. INTRODUCTION

The HYBRID modeling repository collects static and transient physical process models developed within the Integrated Energy Systems (IES) program at Idaho National Laboratory (INL). Primary modeling efforts have centered around transient modeling of various IES subsystems using Modelica. The Modelica [1] language contains a variety of key advantages that are leveraged within the program: acausal equation-based model development, object-oriented, domain-neutral development, fast desktop simulation times, and straightforward access to a base-physics development. The HYBRID repository has been in construction since 2015. As development continues, the number of models grows, making it more difficult for non-developer users to identify specific models. To simplify this process, a single validation and verification (V&V) matrix summarizing available models and their development techniques is established in this report. The goal of this matrix is to consolidate information regarding the available models of the HYBRID repository as well as describe the kinds of data used to develop those models. HYBRID models include systems that are already deployed such as natural gas turbines, Rankine balance of plant (BOP) systems, electric batteries, and large light-water reactors. HYBRID also includes models of some systems that are still in the development phase such as advanced nuclear reactors or thermal energy storage systems.

HYBRID models typically reuse the same component objects across many different models. Pipes, pumps, nuclear kinetics, valves, turbines, heat exchangers, and storage systems are parameterized and not individually developed for given applications. As such, it is important within the HYBRID repository to develop V&V characteristics, as the models are implemented across many subsystems. Validated results within one subsystem model promote confidence in the results of other developed components.

So far, the HYBRID repository has been centered around the Modelica models developed to characterize ramp rates, control methods, and responses to transient conditions. As such, the current status of the V&V matrix will reflect these models. It is a current goal to expand the model repository (and thus this matrix) to include reduced order models (ROMs) of these transient processes as well as add steady-state models. Many steady-state models of IES processes either will be or have been created with a particular focus on IES heat and electricity applications that are not centered on meeting the demands of the electricity grid.

2. VALIDATION AND VERIFICATION TERMINOLOGY

Context is needed to establish the definitions of V&V terminology. The levels of V&V that are used range from reduced to data validation. Note that in the final V&V matrix, first-principle physics and face-validation are combined into one level, published results and code comparison are combined, and data validation has the type of data specifically called out.

Reduced model: Model constructed using reduced algebraic or ordinary differential equations (ODE) relationships that are not derivative of physical conservation equations. An example of this would be a simplified thermal storage system that changes the stored energy content based entirely on the mass flow rates of the charging and discharging fluids while ignoring the nonlinear effects any resulting temperature changes would have on the system.

First-principle physics: This indicates that fundamental conservation laws and peer-reviewed and accepted correlations were the entire basis for a given model. An example of this is the concrete thermal energy storage model. In that model, the temperature distribution is calculated based on thermal conduction within the solid media, and thermal convection between the storage media and the heat transfer fluid. Modelers use accepted, valid methods and observations to ensure that the methods have been appropriately applied.

Face-validation: This indicates that an expert who is not the modeler has observed the results of the constructed model and confirmed that it behaves as expected based on the expert's knowledge within the field. This could be an added step to a first-principle physics model or an evaluation of a specialized model.

Published results verification: Steady-state or dynamic, we consider the comparison with published results to be a contributing piece of V&V, but do consider it to be less robust than validation against internally generated models. The main reasoning for this is the lack of clarifying assumptions often left out of published paper results. Certain physical phenomena may be ignored and undiscussed and, as such, this method of validation begins the validation methods of comparing results.

Steady-state code verification: Comparing with a different steady-state solution code validates the results at steady-state conditions (even for a dynamic model). This is a very important positive result that demonstrates that efficiencies and component sizes are appropriate within the model.

Steady-state data verification: Data are considered superior to code validation. Thus, any experimental or "real-world" data that can be matched gives a higher level of model validation.

Dynamic code verification: Comparison of results with a different dynamic solution from a code is a key level of validation. An example of this validation method would be to analyze a reactor transient and compare the fluid flow values computational fluid dynamics (CFD)-style code.

Dynamic data verification: This is the highest form of validation available. Experiment models are designed specifically to allow for this level of model validation. As many data points as possible should be used during model validation.

2.1 Static and Dynamic Modeling

The reduced model is only considered for static and dynamic modeling types. Experimental models by nature must use more advanced modeling techniques. As such, the descriptions of the different models are described here. An example of the model progression will be shown using a single-pipe concrete thermal energy storage model.

2.1.1 Reduced Model

Reduced models as primary models should be considered a simplified algebraic or ODE relationship, mapping an input space to an output space without also using primary physics development. These kinds of models are typically avoided within HYBRID, as primary modeling concerns regard dynamic analysis of complex systems, necessitating the use of primary physics modeling. A good use of this modeling technique can be reserved for boundary condition modeling evaluation. An example might be an assumed chemical process conversion rate using input mass flow rate, such as an ammonia production rate from an IES plant, without modeling the internal processes and operational characteristics of that ammonia plant.

Through this chapter, the HYBRID model of concrete thermal energy storage (CTES) will be used as an example. Observing the changes in Figure 1, it is possible to guess how a simplified model might miss any underlying effects. For instance, if the net energy stored was a simplified model as a linear combination of net charging mass minusnet discharging mass (such as in equation 1), the overall energy capture might be determined. However, the specific curves and changes within the conservation equation-based system would be missed due to the model's simplicity.

$$(E\_stored = \Delta h\_charge\ m\_charge - \Delta h\_discharge\ m\_discharge) \tag{1}$$

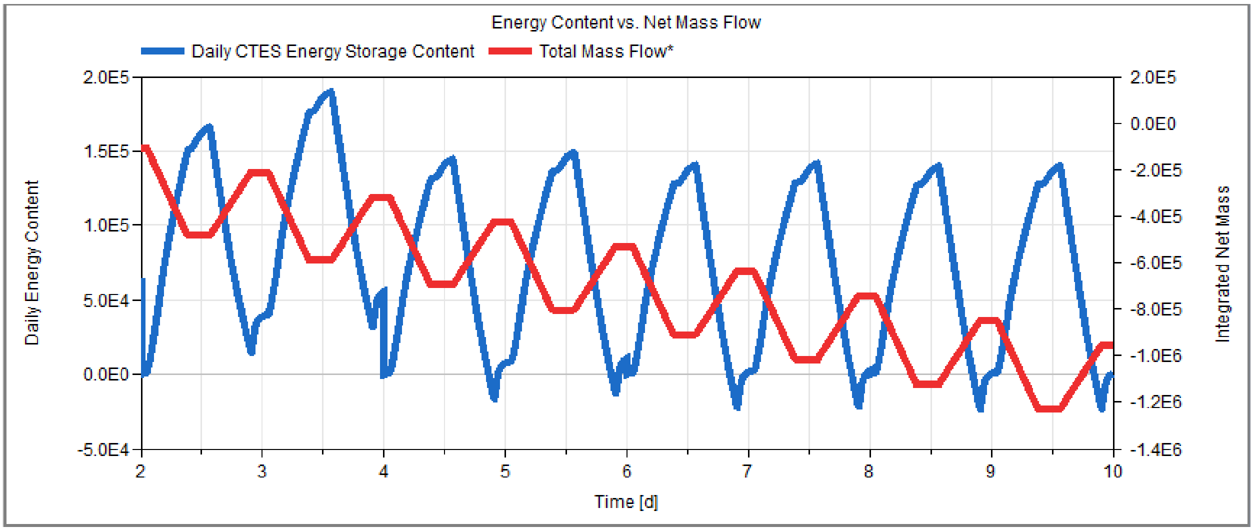

Figure 1. Total energy stored versus net mass within a single-pipe CTES system.

These results demonstrate that the system characteristics are not captured by a simplified or reduced model, and in many cases this is an impetus for first-principle physics and face-validated models.

2.1.2 First-principle Physics and Face-validation

First-principle physics modeling is the primary modeling technique used within HYBRID. This modeling technique is implemented through application of physical conservation equations (conservation of mass, momentum, and energy) within individual components. These models add closure relationships that may be algebraic in nature as appropriate (e.g., heat transfer coefficients, pressure loss due to friction, neutron kinetics) and widely used within physical modeling efforts. This level of model construction is initially considered to be a higher level of V&V. All nuclear reactor concept models built within HYBRID use this method to describe the physical system operation. This type of modeling should be validated if data become available, either through another modeling effort or through experiment. A slightly higher level of validation exists with these models wherein an expert within the field of the developed model confirms the behavior of the model that was developed.

Continuing from the example of the simplified model, Figure 2 shows the temperature results within the single-pipe simulation using steam charging and discharging of the system. These temperatures show the result of a nonlinear heat exchange between the heat transfer fluid and the concrete system (observable through the highly nonlinear temperature lines). All operational characteristics align with expert expectations of this system, interfacing with a latent-heat-based heat transfer fluid.

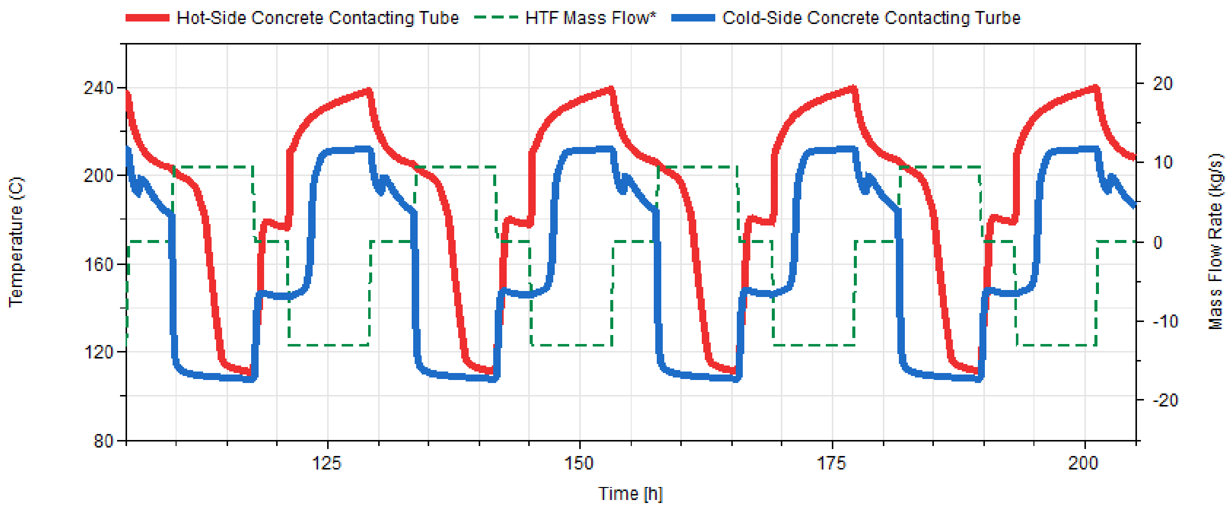

Figure 2. Single-pipe CTES results of a periodic charge and discharge cycle. Hot end and cold end concrete temperatures are plotted.

2.1.3 Validation through Comparison

Validation can occur for some models through comparison with other modeling results. These comparisons can comed from two sources: other accessible models and published results. Occasionally, published results and data validation can be considered identical if the published results are physically demonstrated data. One method that might be used for validation through comparison would be a CFD code to model the CTES system. This activity has not been completed. As such, the CTES example shown throughout the current chapter continues in the next section.

2.1.4 Data Validation

Data validation is considered the highest form of model validation: using physical information from a deployed process to verify the simulation values from a given model. This type of validation requires a physically built system and thus may not be an option for certain models such as models of advanced reactor concepts.

As seen in Figure 3, there are physical results data from a demonstration run of a CTES system constructed by EnergyNest [2]. These data can be used to compare with the simulation results of the HYBRID model that has been constructed. Due to some model constraints, this particular dataset cannot be directly modeled within HYBRID. However, many of the future comparison principles still remain. The shapes of the mass flow rate curves compared in Figure 2 and Figure 3 show that the overall demonstration plan is consistent. Alternating periods of charging and discharging are used to show the cycle behavior of the CTES system. The hot temperature curves compared in Figure 2 and Figure 3 show a consistent shape during the charging and discharging phases, a very positive result for the HYBRID model. The shape of the cold temperature curves does not match quite as identically, although one reason that might explain the difference is apparent: the published demonstration results are from a system that used a thermal oil as a heat transfer fluid into and out of the system, resulting in a system where no phase-change occurred. The heat transfer fluid used in the HYBRID model that produced the results in Figure 2 was water on both sides, so that steam condenses and water boils during charging and discharging. This led to the temperature plateaus distinctly observed in Figure 2, but not in Figure 3. As of this publication, this is a model constraint that will need to be addressed to better match the experimental results and raise the V&V level of this model to data validation from the current face-validation.

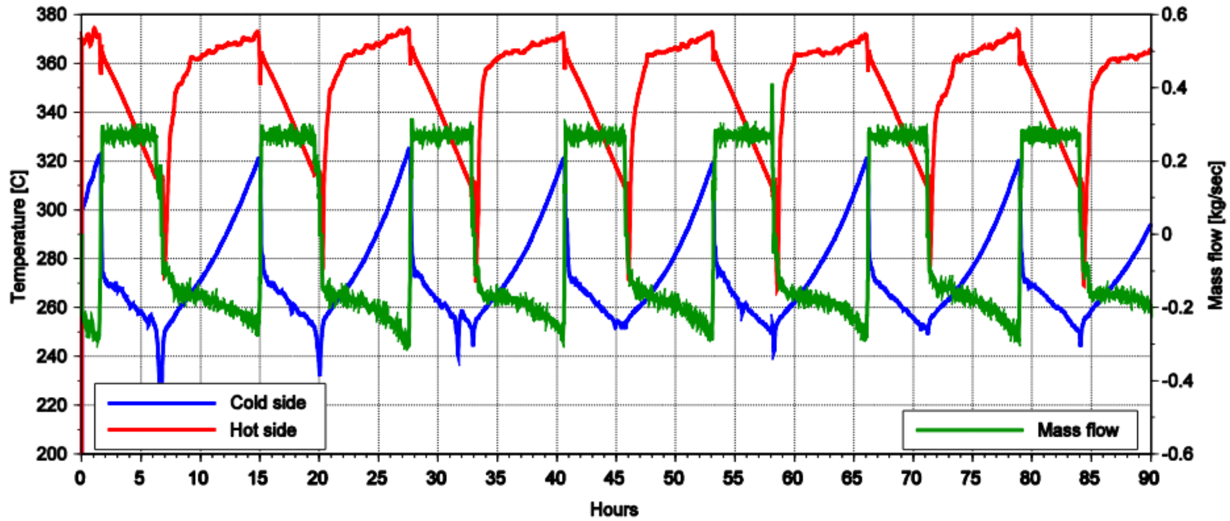

Figure 3. Physical demonstration results of a concrete TES system [2].

While these results cannot be used to completely validate the current HYBRID model, they do lend support to the notion that the characteristics of the system are well-captured. Through additional model enhancements, these data can be used for V&V. For V&V efforts, more HYBRID models with physical data should continue, with more alterations to adapt the HYBRID model and more accurately portray the specific system that produced the data. HYBRID models are typically constructed within the context of a single application so certain modeling choices seen as features at the time of model construction may need to be adjusted to accommodate the physical characteristics of the system that produces validation data. This includes steam charging and discharging for the CTES model, which was built to study load-following of a light-water reactor system using steam bypass to charge the CTES, with steam production introduced into the turbogenerator system when discharging the CTES).

2.2 Experimental Modeling

Experiment V&V has fewer categories because of the nature of the modeling efforts. Instead of the four levels of dynamic and static modeling, there are only three V&V categories for experimental modeling: first-principle physics, code-to-code comparison, and data verification. For now, the only experimental modeling within HYBRID focuses on the subsystems of the Dynamic Energy Transport and Integration Laboratory including the Microreactor Agile Non-nuclear Experimental Testbed (MAGNET) and the Thermal Energy Distribution System (TEDS). TEDS produced some data in 2021 that were used to validate the HYBRID model, and current fiscal year efforts include extending that validation and adding validation for the MAGNET model [3].

2.2.1 First-principle Physics

The first-principle physics models are mainly produced during the experimental design phase to assist with prediction and physical design. The physics as understood are implemented in order to predict future conditions. In many cases, these predictions can then be used to inform or confirm design decisions made for laboratory experiments.

2.2.2 Code-to-code Comparison

A code-to-code comparison may occur in experimental modeling, especially if multiple tools are used in the design process. One example of this would be steady-state and highly detailed CFD models comparing various results of a dynamic systems code.

2.2.3 Data Verification

Data verification is the process of V&V using experimentally produced data to compare against results of a matching simulation. The workflow for this process using HYBRID and RAVEN has been established and will continue to be demonstrated in future work.

3. EXAMPLE TYPES

This section includes a brief discussion on the example types that currently exist within the 'devel' branch of HYBRID. Examples that operate are important as they present appropriate uses of developed models within the context of intended use.

3.1 Individual Example

Individual examples demonstrate the operation of a subsystem independently. This is typically done using boundary conditions at the external interfaces of the subsystem. For example, a primary reactor core loop, such as the system seen in Figure 4 and Figure 5 might have a simulated feedwater flow source into the primary heat exchanger at the appropriate flow conditions. The four-loop pressurized water reactor (PWR) is used as an example to demonstrate this concept. Screengrabs show the examples included in the primary development branch of HYBRID.

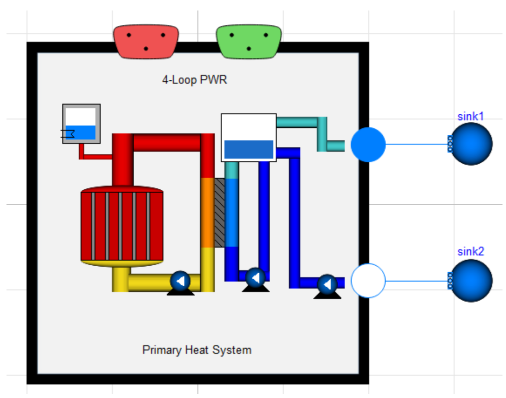

Figure 4. Standalone model of the four-loop PWR system. This is a typical individual example: one in which boundary conditions connected at the edge of the subsystem model are used to check the operability of the subsystem model.

Figure 5 shows the full four-loop PWR subsystem model at the detailed level. The primary flow loop is on the left side of the image and includes the reactor core, piping, pressurizer, and coolant flow pumps. The right side of the image shows the components interfacing with the steam production system, including a steam drum boiler. The steam generator near the middle of the image is the heat transfer connection point between the primary and secondary sides of the nuclear reactor. This representation of a subsystem shows how an independent subsystem should be constructed: to be complete with just boundary conditions defining the interface points to the external systems. In the case of a nuclear reactor, the boundary conditions needed are a source of feedwater and a boundary condition sink for steam to flow to, as was seen in Figure 4.

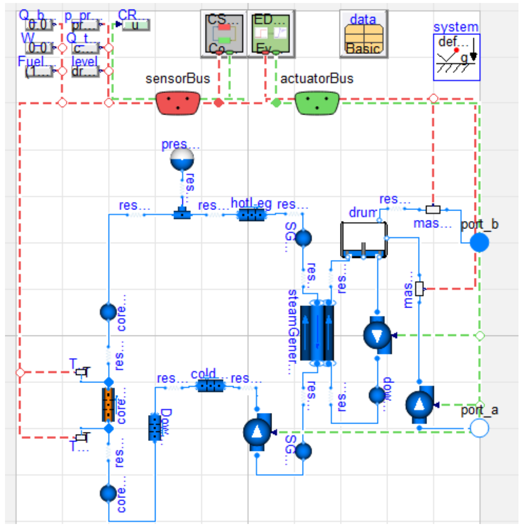

Figure 5. Model of the four-loop PWR when opened as a single subsystem.

3.2 Integrated Example

An integrated example uses a subsystem within an integrated energy system environment. A typical integrated system within HYBRID incorporates a nuclear steam supply system, balance of plant, energy storage, and a heat application. IES examples contained within HYBRID are associated with specific past use cases. Figure 6 shows an IES example within the primary development branch of HYBRID that contains the four-loop PWR subsystem. These integrated systems are typically the source of simulation results for various publications from the IES team.

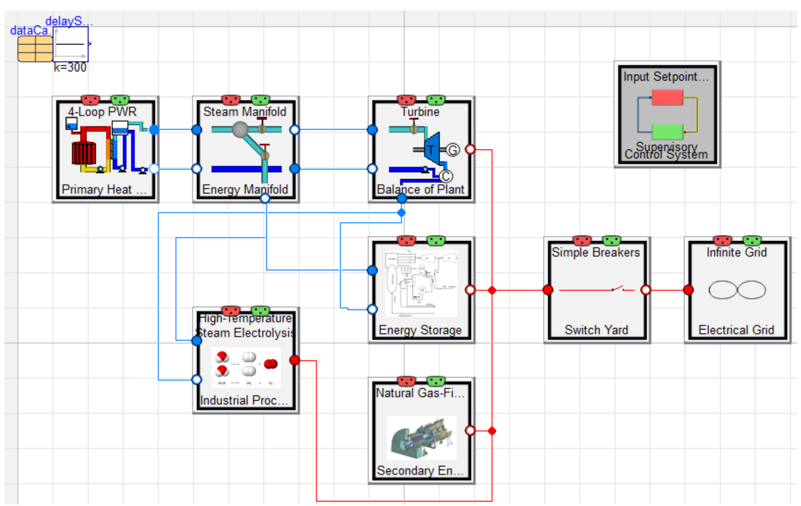

Figure 6. Integrated example that includes the four-loop PWR system. This full IES contains many components combining to flexibly produce energy across the energy park.

3.3 ROM Generation

An ROM is trained from physical models in HYBRID using repeated simulation of a particular ROM method. Risk-Analysis Virtual Environment (RAVEN) generates these ROMs using several methods, including a highly relevant method to HYBRID models called dynamic mode decomposition with control (DMDc) [4], which can create surrogate models of a dynamic system that operates using control schemes.

Producing ROMs can have multiple benefits, including portability to interface with models generated by other codes, faster simulation times, and direct input-output mapping. DMDc is a method of particular interest to the IES team as nearly all IES subsystem components include control systems to meet certain setpoints through changing certain components. Controlled components include valves, pumps, compressors, blowers, mass flow sources, heaters, coolers, and control rods. As more ROMs are generated in ongoing work, these will be added to the HYBRID repository.

4. CURRENT HYBRID V&V MATRIX

The current status of the HYBRID repository is shown in **Error! Reference source not found.**. Information regarding the current models is categorized generally as: nuclear generators, thermal energy storage systems, experimental systems, steam applications, and additional IES components (electrical transmission models, alternative heat sources, thermal distribution).

Table 1. V&V matrix for the current model set within HYBRID, focusing on the transient physical models: nuclear generators, thermal energy storage, experimental systems, steam applications, and additional IES components. Published documents contain results produced from the model, while reference documents indicate materials used to generate a given model.

	Subsystem Name	V&V	Example Type	ROM generated	Steady-state model	Published documents	Public Reference documents	Nominal Conditions, Notable Limitations
Nuclear Generators	Four-loop PWR	Face	Integrated	–	–	doi: 10.2172/1569271	Systems Summary of a Westinghouse PWR Nuclear Power Plant 1984 “PWR Description,” Jacopo Buongiorno	3400 MW(t), Steam: 1750 kg/s, 69 bar, 285°C
	Small modular IPWR	Data: steady state	Integrated	–	–	INL/CON-16-39032	https://aris.iaea.org/PDF/NuScale.pdf doi: 10.1016/j.desal.2014.02.023	160 MW(t), Steam: 35 bar, 300°C, 75 kg/s
	Small modular natural circulation IPWR	Data: steady state	Integrated	–	–	doi 10.2172/1569288 doi:10.1080/00295450.2020.1781497 doi:10.1016/j.apenergy.2022.118800 doi: 10.2172/1890160	NuScale Standard Plant Design Certification Application	200 MW(t), Steam: 35 bar, 310°C, 84 kg/s
	High Temperature Gas Reactor (Pebble Bed & Prismatic separate)	Data: Transient	Integrated	–	—	doi: 10.2172/1890160 doi: 10.2172/1881858 doi: 10.2172/1880089 doi: 10.2172/1890160	doi: 10.1016/j.nucengdes.2017.11.041	130 MW(t), Steam: 140 bar, 540°C, 50 kg/s
	Molten Salt Reactor	Physics	Individual	–	–	INL/RPT-23-74700 (DOI coming)	–	750 MW(t) Steam: 540°C, 289 kg/s
	Sodium Fast Reactor	Physics	Individual	–	–	doi: 10.2172/1881858	–	BOP under construction
Thermal Energy	Solid Media TES	Face	Integrated	–		doi: 10.1016/j.est.2022.104387 doi: 10.1016/j.apenergy.2022.118800 doi: 10.2172/1787041	doi: 10.1063/1.4984432	Nominally concrete, requires steam
	2-tank TES	Face	Integrated	–	–	doi: 10.2172/1468648 doi: 10.2172/1880089 doi: 10.2172/1890160	–	Molten salt
	Thermocline TES	Physics, some data	Integrated	–	–	doi: 10.2172/1668777 doi: 10.2172/1836100 doi: 10.2172/1787041	–	Thermal oil
	Latent heat TES	Physics, some data	Individual	–	–	doi: 10.2172/1787041	–	–
	Battery storage	Physics	Integrated	X	–	INL/MIS-20-60624	–	–

	Subsystem Name	V&V	Example Type	ROM generated	Steady-state model	Published documents	Public Reference documents	Nominal Conditions, Notable Limitations
	Compressed air	Physics	Individual	–	–	doi: 10.2172/1880089	–	Single-mode operation
Experimental systems	TEDS loop	Physics, some data	Individual, Integrated	–	–	doi: 10.2172/1668777 doi: 10.2172/1836100	–	–
	MAGNET loop	Physics	Individual, Integrated	–	–	INL/EXT-22-02188	–	–
Steam Applications	Reverse osmosis desalination	Data: steady state	Integrated	–	–	doi: 10.2172/1468648 doi: 10.2172/1244626	–	–
	High temperature steam electrolysis	Data: steady state	Integrated	–	–	INL/EXT-16-40305 doi: 10.2172/1569271	doi: 10.1016/j.jpowsour.2006.12.081 doi: 10.1016/j.ijhydene.2012.12.086 doi: 10.2172/1513461	–
	HTSE 'experimental'	Face	Individual	—	–	INL/RPT-22-70396	–	–
	Multi-effect evaporator	Physics	Integrated	–	–	–	Upcoming	–
	Heat recovery steam generator	Physics	Integrated	–	–	–	Upcoming	–
	Single-stage balance of plant	Face	Integrated	–	–	Many	–	–
	Two-stage balance of plant	Face	Integrated	–	–	doi: 10.2172/1890160	–	–
	Three-stage balance of plant	Face	Integrated	–	–	INL/RPT-23-74700 (DOI coming)	–	–
	Stage-by-stage balance of plant	Physics	Integrated	–	–	doi: 10.1016/j.apenergy.2022.118800	–	–
Additional IES Components	Steam manifold	Physics	Integrated	–	–	Many	–	–
	Switchyard	Physics	Integrated	–	–	Many	–	–
	Electric grid	Physics	Integrated	–	–	Many	–	–
	Natural gas turbine	Face	Integrated	X		INL/EXT-16-40305	–	–

5. CONCLUSIONS

A V&V matrix for public use was developed for the HYBRID repository. As the repository continues to develop, additional models and publications will be added to this matrix, which will be updated periodically on public-facing websites and likely should be annually re-published in a fully documented form.

Additional V&V efforts should be made across as many models as possible for the HYBRID repository. The multi-domain and single-machine modeling capabilities of HYBRID can allow for powerful use of the repository across many industries to analyze potential IES. As many models rely on similar components, every V&V demonstration not only increases confidence in results from that particular model but can also be extended across the HYBRID repository.

6. ACKNOWLEDGEMENTS

This work was supported by the IES program at INL under DOE Operations contract no. DE-AC07-05ID14517.

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Table 2. V&V matrix for the current model set within HYBRID, focusing on the transient physical models: nuclear generators, thermal energy storage, experimental systems, steam applications, and additional IES components. Published documents contain results produced from the model, while reference documents indicate materials used to generate a given model.

	Subsystem Name	V&V	Example Type	ROM generated	Steady-state model	Nominal Conditions, Notable Limitations
Nuclear Generators	Four-loop PWR	Face	Integrated	–	–	3400 MW(t), Steam: 1750 kg/s, 69 bar, 285°C
	Small modular IPWR	Data: steady state	Integrated	–	–	160 MW(t), Steam: 35 bar, 300°C, 75 kg/s
	Small modular natural circulation IPWR	Data: steady state	Integrated	–	–	200 MW(t), Steam: 35 bar, 310°C, 84 kg/s
	High Temperature Gas Reactor (Pebble Bed & Prismatic separate)	Data: Transient	Integrated	–	—	130 MW(t), Steam: 140 bar, 540°C, 50 kg/s
	Molten Salt Reactor	Physics	Individual	–	–	750 MW(t) Steam: 540°C, 289 kg/s
	Sodium Fast Reactor	Physics	Individual	–	–	BOP under construction
Thermal Energy	Solid Media TES	Face	Integrated	–		Nominally concrete, requires steam
	2-tank TES	Face	Integrated	–	–	Molten salt
	Thermocline TES	Physics, some data	Integrated	–	–	Thermal oil
	Latent heat TES	Physics, some data	Individual	–	–	–
	Battery storage	Physics	Integrated	X	–	–
	Compressed air	Physics	Individual	–	–	Single-mode operation
Experimental	TEDS loop	Physics, some data	Individual, Integrated	–	–	–
	MAGNET loop	Physics	Individual, Integrated	–	–	–
Steam Applications	Reverse osmosis desalination	Data: steady state	Integrated	–	–	–
	High temperature steam electrolysis	Data: steady state	Integrated	–	–	–
	HTSE ‘experimental’	Face	Individual	—	–	–
	Multi-effect evaporator	Physics	Integrated	–	–	–
	Heat recovery steam generator	Physics	Integrated	–	–	–
	Single-stage balance of plant	Face	Integrated	–	–	–

	Subsystem Name	V&V	Example Type	ROM generated	Steady-state model	Nominal Conditions, Notable Limitations
	Two-stage balance of plant	Face	Integrated	–	–	–
	Three-stage balance of plant	Face	Integrated	–	–	–
	Stage-by-stage balance of plant	Physics	Integrated	–	–	–
Additional IES	Steam manifold	Physics	Integrated	–	–	–
	Switchyard	Physics	Integrated	–	–	–
	Electric grid	Physics	Integrated	–	–	–
	Natural gas turbine	Face	Integrated	X		–