Value-Driven Design and Sensitivity Analysis of Hybrid Energy Systems using Surrogate Modeling

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Wenbo Du, Humberto E. Garcia, William R. Binder, Christiaan J. J. Paredis

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Wenbo Du[1], Humberto E. Garcia[1,*], William R. Binder[2], Christiaan J. J. Paredis[2]

[1]Idaho National Laboratory, Idaho Falls, ID, USA
[2]Georgia Institute of Technology, Atlanta, GA, USA
[*]Email: humberto.garcia@inl.gov

Abstract—**A surrogate modeling and analysis methodology is applied to study dynamic hybrid energy systems (HES). The effect of battery size on the smoothing of variability in renewable energy generation is investigated. Global sensitivity indices calculated using surrogate models show the relative sensitivity of system variability to dynamic properties of key components. A value maximization approach is used to consider the tradeoff between system variability and required battery size. Results are found to be highly sensitive to the renewable power profile considered, demonstrating the importance of accurate renewable resource modeling and prediction. The documented computational framework and preliminary results represent an important step towards a comprehensive methodology for HES evaluation, design, and optimization.**

Keywords-hybrid energy systems; renewable energy; value maximization; surrogate modeling; dynamic modeling and simulation; sensitivity analysis

I. INTRODUCTION

Renewable energy technologies have attracted significant attention in recent years due to a variety of factors, including sustainability concerns and environmental impacts of fossil resources. A major challenge facing renewable technologies, such as wind and solar power, is their unpredictable, intermittent, and uncontrollable nature. The large degree of variability in renewable sources makes them inadequate for directly meeting typical energy demand profiles. One method for mitigating the effects of variability is to integrate renewable sources into the grid via hybrid energy systems (HES). HES combine multiple energy resources within a single system and have been shown to be capable of achieving superior flexibility and cost efficiency compared to traditional systems [1,2]. However, the integration of multiple energy resources increases the complexity of the system, making the operation and performance of HES accordingly more difficult to model. Consequently, the optimal design and operation of HES remain open challenges.

HES potentially offer many advantages, but realizing these advantages requires the development and utilization of appropriate modeling and simulation tools. Previous work has made considerable progress by establishing a computational framework for HES using dynamic models in conjunction with optimization tools [2]. However, significant gaps in understanding the dynamic behavior HES remain. For example, the optimization results in [2] impose linear constraints to mimic the cost of increasing the battery size, but do not calculate the battery size directly – a quantity of greater physical significance. The optimization results also do not provide information about the relative sensitivity of the system performance to specific system components, and thus give no indication of the relative importance of their design. Finally, the assumption of a fixed renewable energy generation profile ignores a substantial source of uncertainty and variability in the HES model. We seek to address these deficiencies by extending the established computational framework with additional tools and capabilities. Therefore, we define the following objectives in the present work:

1. Integrate surrogate modeling and analysis tools with dynamic HES simulations to efficiently model system performance;

2. Apply surrogate modeling to quantify the relative sensitivity of the system to the dynamic properties of specific components;

3. Assess the relative costs of designing HES to minimize variability versus battery size; and

4. Examine the impact of varying renewable energy generation profiles on system performance.

This paper is organized as follows. We first introduce the computational methodology used in the work, including an overview of the HES configuration being modeled and the surrogate modeling and analysis tools. We then apply these tools to study the effect of battery size on system variability, the relative impact of the various subsystem dynamics using global sensitivity analysis (GSA), and the tradeoff between two key design objectives. We conclude the paper with a summary of the key findings and a discussion of important ongoing and future research directions related to HES modeling, design, evaluation, and optimization.

II. METHODOLOGY

A. HES Model

In this section, we provide a high-level overview of the HES model considered; interested readers may wish to consult [2] for further details. A schematic diagram for the HES model of interest is illustrated in Fig. 1. This HES configuration includes a high temperature gas reactor (HTGR) and a Brayton helium closed cycle plant for the baseload generation. A series of wind turbines comprise the renewable generation, whose electrical power input to the HES is regulated by an electrical

storage element (battery). Note that while we consider wind as the renewable generation technology, the methodology is sufficiently flexible to allow additional renewable resources such as concentrated solar-thermal to be included. Two distribution centers for helium and electricity regulate the distribution of each resource to the grid and to a high temperature steam electrolysis (HTSE) subsystem, where chemical products (hydrogen and oxygen) are produced.

Since the system receives multiple energy inputs (baseload and renewable generation) and outputs multiple products (electricity and chemicals), this is an example of a Multiple Input Multiple Output (MIMO) system, which can offer significant advantages in flexibility, utilization, economic opportunities, and efficiency over single-output configurations [1]. For computational simplicity, the HTGR, Brayton plant, and HTSE subsystems are modeled by linear transfer functions with lumped quantities to account for sizing, efficiency, and unit conversions. The gains and time constants are obtained from empirical data and steady-state analysis. Note that the model in Fig. 1 contains both energy flows (shown as solid blue arrows) and information flows (dotted red arrows). Energy flows can further be divided into thermal (in the form of heated helium) and electrical energy flows.
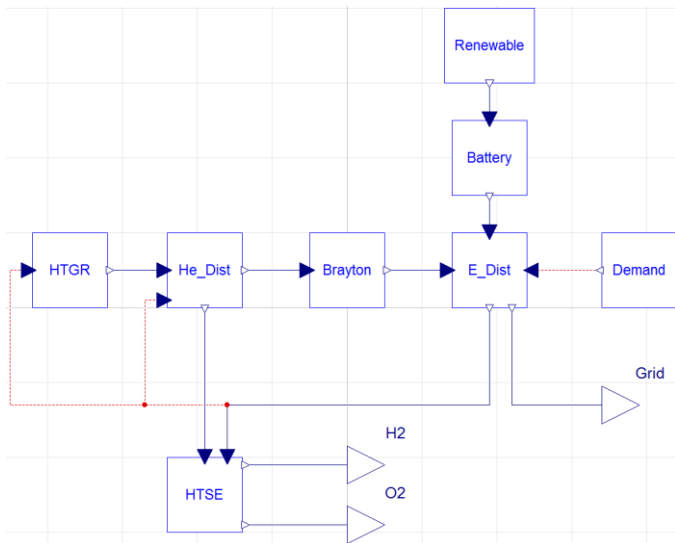

Figure 1.   Block diagram of HES model

The conversion of thermal to electrical energy occurs in the power cycle plant, where high temperature helium from the helium distribution center is used to produce electricity via a Brayton closed cycle. The electricity produced by the Brayton power plant is then combined with electricity from the renewable source and battery, and dynamically distributed to the grid and HTSE subsystem according to the demand. For simplicity, a constant demand profile is assumed, and the HTGR and Brayton plant are sized to ensure that the demand can be satisfied by the baseload generation alone. Therefore, the energy flows are distributed such that the demand is satisfied exactly (a perfect controller is assumed) when there is an excess in electrical energy due to the presence of renewables. Meanwhile, the helium distribution center, which receives heated helium from the HTGR, also dynamically

distributes thermal energy to the HTSE in accordance with the electrical energy flows. These assumptions ensure that the HTSE unit does not need to shut down, and will produce hydrogen and oxygen at a rate that correlates strongly with the renewable power profile.

The renewable generation is provided by a set of identical wind turbines modeled with wind speed data collected for a site in Wyoming. Turbine power is assumed to be zero below a cut-in speed of 3 m/s and above a cut-out speed of 25 m/s. Between the rated speed of 14 m/s and the cut-out speed the turbine is assumed to deliver the rated power of 2 MW, and between the cut-in and rated speed the power is assumed to follow a cubic law. The rated power corresponds to a turbine located at an altitude of 1500 m with a diameter of 50 m and overall efficiency of 55%.

B. Surrogate Modeling and Analysis

Surrogate modeling, also known as response surface modeling or metamodeling, is a technique for constructing reduced order models of engineering systems based on the concept of fitting surrogate functions to approximate the true output of a model. Surrogate models are constructed from the results of a predetermined set of simulations designed to sample the parameter space (design of experiments or DOE), and have been previously utilized to study a variety of engineering problems [3, 4]. An important advantage of the surrogate modeling approach is a significant reduction in simulation time compared to the original model, since most classes of surrogate models are analytically defined. This property makes surrogate modeling effective for applications requiring a large number of simulation samples, such as GSA [5, 6] and optimization [7, 8].

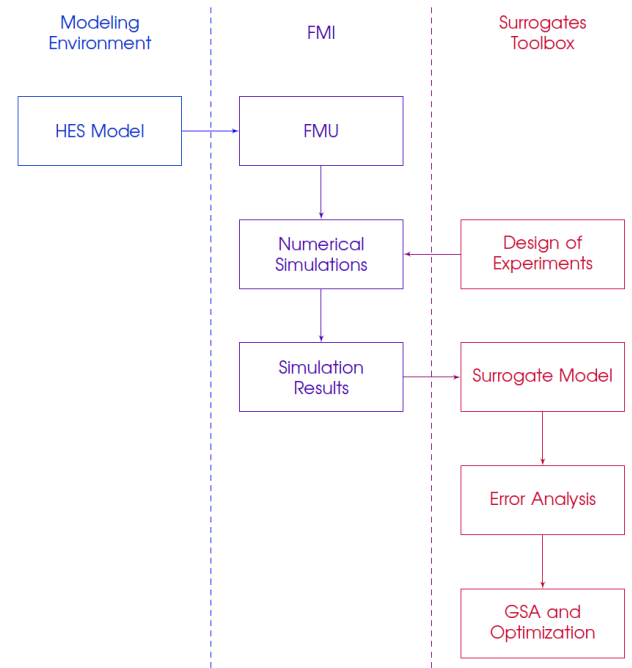A diagram of the surrogate modeling and analysis process is shown in Fig. 2.

Figure 2.   Surrogate modeling and analysis methodology

We note that our analysis involves the use of three computational environments. The HES model is constructed using the Modelica modeling language and simulated using a commercial package called Dymola. Surrogate modeling and analysis is performed in MATLAB using an established surrogate modeling toolbox. An interface is needed to allow the surrogate modeling tools to setup and modify the HES simulations according to the DOE. For this purpose, we use Functional Mockup Interface (FMI) for model exchange, which builds a Functional Mockup Unit (FMU) of the Modelica-based HES model [9].

To sample the parameter space, we employ an approach combining Latin Hypercube Sampling (LHS) [10] and Halton Sequence (HS) [11] methods for the DOE. After running the simulations according to the DOE, several classes of surrogate models are possible [12]. As we expect the parameter space to be continuous and smooth, we select polynomial response surface (PRS) models for simplicity, while recognizing that other methods such as kriging may be more suitable for discontinuous or highly nonlinear problems [13]. For the error assessment, we consider two standard error measures: the prediction error sum of squares (PRESS) and coefficient of determination (R^2) [14]. For GSA, we apply Sobol's method of decomposition using Monte Carlo simulations [15].

III. PROBLEM FORMULATION AND RESULTS

Wind velocity data are sampled at time intervals of 600 seconds over a one-year period. For the calculation of battery size and surrogate modeling, a two-week period beginning on the 311st day of the year is selected for all simulations. We select the same sampling intervals in our simulation results to avoid needing to interpolate between data points. Therefore, all simulations are conducted for a time period of two weeks (1.21×10^6 seconds) with a total of 2017 time steps. The wind velocity and corresponding turbine power profiles for this period are shown in Fig. 3.
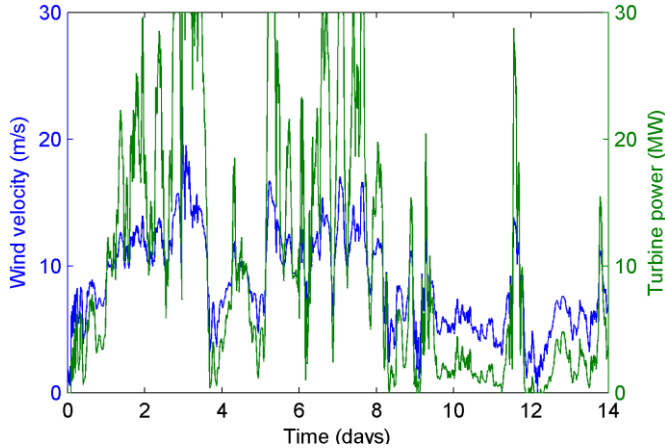

Figure 3. Wind velociy and turbine power profiles for two week period

Note the high degree of variability in the wind velocity, which is responsible for introducing undesired variability into the HES. We model the renewable component of the HES as a set of 15 identical 2 MW wind turbines, for a total rated power of 30 MW. The turbines are assumed to operate independently and are located sufficiently far apart to not experience interference.

For all simulations, the HTGR provides a constant power input of 300 MWt (corresponding to 135 MWe following the Brayton plant). The grid demand is assumed to be a constant value of 100 MWe. As previously mentioned, the baseload is intentionally oversized to avoid a situation where the HTSE needs to be shut down, as this is a highly undesirable situation in the operation of large energy systems. The HTSE process is assumed to occur very quickly, with a time constant of 1 second, and oxygen and hydrogen are produced in a 7.94:1 ratio by mass.

A. Calculation of Battery Size

It has already been established that, in the absence of constraints, a large time constant associated with the battery is preferred, as it helps smooth out variability due to renewables [2]. However, it is also known that a larger time constant requires a larger storage capacity battery to satisfy the charging and discharging dynamics to smooth out the variability. Clearly, a proper calculation of the required battery size is needed as a constraint when optimizing the design of the HES. The effect of varying the battery time constant can be observed in Fig. 4, which plots the power profiles of the renewable source alone (blue), and of the renewable and battery arrangement (red). Note that the time constant corresponding to the battery is used to characterize the smoothing effect that the battery would have on the electricity delivered by a renewable and battery arrangement, and should not be confused with the charge or discharge rate of the battery.
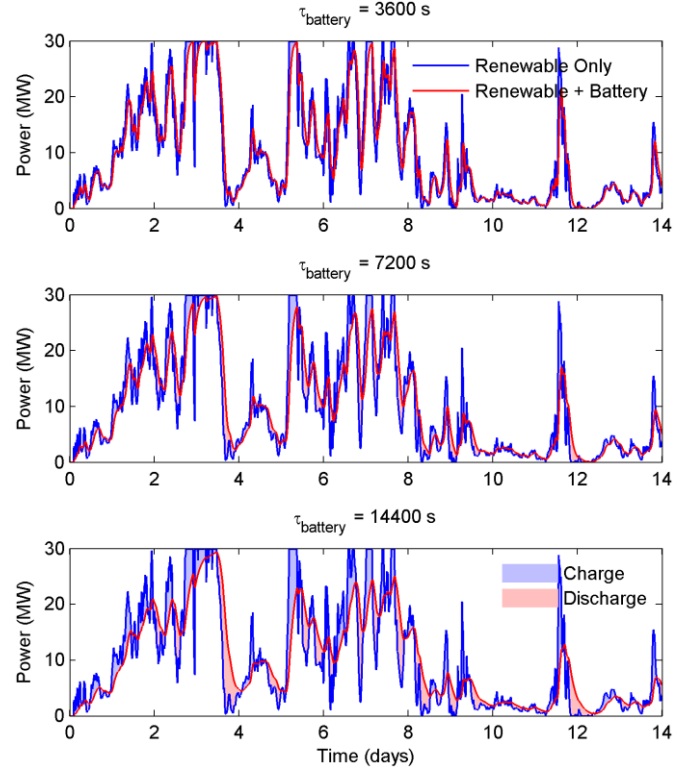

Figure 4. Impact of battery time constant on charge and discharge

The difference in instantaneous power output between the two power profiles is the power that the battery must provide as discharge or accept to charge itself. The shaded area between the curves represents the total amount of energy during a single charge or discharge period, and the largest single contiguous area is the minimum energy storage capacity required for the battery to meet the specified smoothed profiles for renewable energy generation.

In addition to the required storage capacity, the maximum required power is also a useful metric to consider. This is because battery packs consist of a large number of cell arrays arranged in parallel, which in turn contain multiple individual cells arranged in series. The total number of cells in the battery pack determines the size, but the numbers of cells in series and arrays in parallel are dictated by the maximum required power. The maximum power rate can be determined by computing the instantaneous value of the difference between the renewable and renewable-plus-battery arrangement, and the corresponding profile is plotted in Fig. 5.
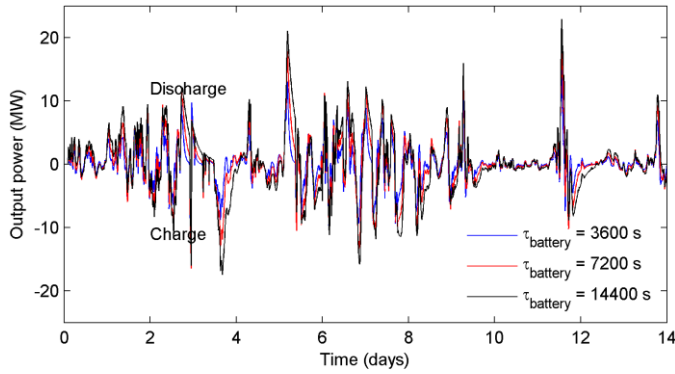

Figure 5. Charge and discharge profiles for three battery time constants

Using the methods outlined above, the maximum charge and discharge power rates and required energy storage values are calculated and reported in Table I. These results confirm that the necessary battery size increases substantially with the battery time constant, and that the storage size is more sensitive to this effect than the maximum power is. It is also observed that the battery has greater requirements for discharge than for charge. These findings can significantly improve the value HES optimization when properly considered as design constraints.

TABLE I. BATTERY SIZE REQUIREMENTS

Time constant (s)	3600	7200	14400
Max. charge power (MW)	13.7	16.4	17.4
Max. discharge power (MW)	16.6	20.2	22.9
Req. charge storage (MW-hr)	26.4	48.6	75.1
Req. discharge storage (MW-hr)	27.3	54.8	99.3

B. Surrogate Modeling and Sensitivity Analysis

To reduce the total computational cost of the process, we apply GSA to a surrogate model. We consider three variables in the surrogate model: the time constants for the battery, HTGR, and Brayton plant. The objective function considered is the total time-integrated variability in electrical power entering the HTSE, calculated in a similar manner to the required battery size in section A. For the DOE, 20 LHS and 20 HS points are selected, for a total of 40 samples. Halton bases of 7, 17, and 23 are selected for the HS samples. Lower and upper bounds on all three time constants are varied geometrically around nominal values of 7200, 450, and 4 seconds for the battery, HTGR, and Brayton cycle respectively.

A 3rd order PRS is found to have normalized RMS PRESS of about 1.3% and R^2 = 0.999, which we consider adequate to obtain meaningful results with GSA. By inspection, the HTSE electrical power variability is found to increase with increasing HTGR and Brayton cycle time constants, but decrease with increasing battery time constant. This is consistent with the trends observed in the unconstrained optimization case in [2]. Fig. 6 shows the main and total global sensitivity indices calculated using Sobol's method.
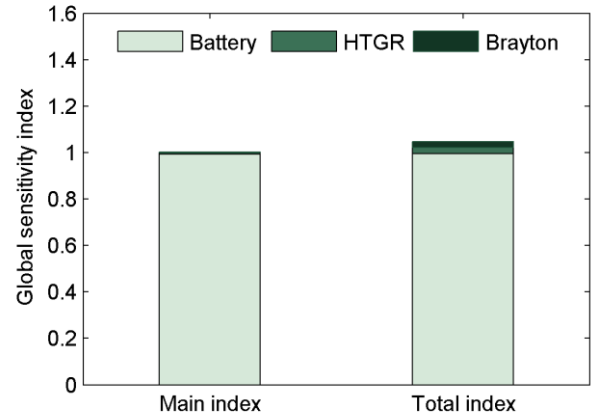

Figure 6. Main and total sensitivity indices

A total of 50,000 Monte Carlo simulations with the surrogate model are used, and subsequent trials confirm the convergence of the results. We observe that the HTSE variability is dominated by the effect of the battery, further highlighting the importance of accurately evaluating and optimizing the battery size. It should be noted that, numerically, the battery should be expected have the greatest impact on system variability, given that its time constant has the greatest range to vary within the parameter space. However, given that the ranges are selected to be consistent with physical constraints on the systems, the GSA results confirm the importance of properly designing system components with the greatest variation in sizing and dynamic operation.

C. Value-Driven Design

Previous results have assumed a certain wind profile for the renewable energy source and focused on a single objective of study (i.e., minimizing the variability in HTSE electrical power). Here we consider the effect of varying the wind power, in the context of designing the system to maximize value. The rationale behind minimizing variability is to reduce operating

costs associated with excessive wear on the system components. However, our findings that the required battery storage size increases with time constant show that it is also important to consider capital costs. A value maximization problem is thus formulated, in which the value function depends on two attributes: minimizing variability to reduce maintenance costs, and minimizing battery size to reduce capital costs. To reach a reasonable compromise between these two attributes, one could minimize the total cost of ownership, which takes both the maintenance and capital costs into account [16]. We are also interested in investigating how the relationship between the two attributes varies with the wind profile.

Two 2-week periods, beginning on the 169th and 311st days of the year, are selected and shown in Fig. 7.
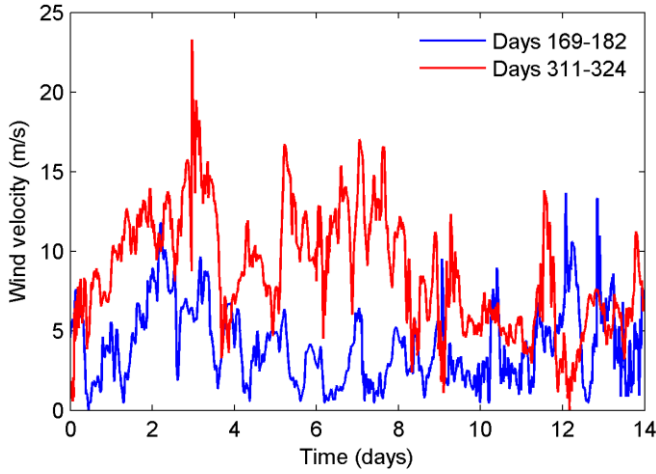

Figure 7. Two 2-week wind velocity profiles

We note that the latter period exhibits much greater variation and total wind velocity, and can be expected to lead to greater HTSE variability. This is confirmed in Fig. 8, which plots the value attributes corresponding to the two wind profiles.
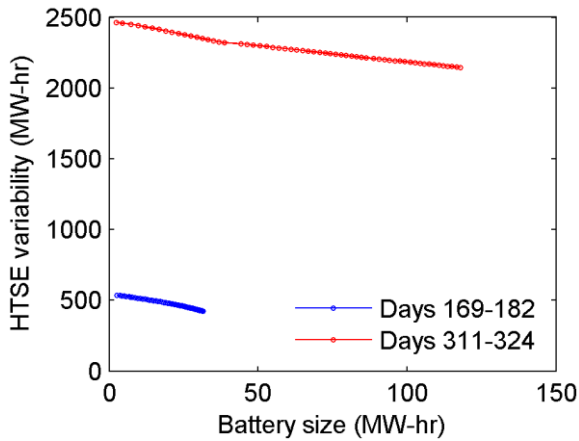

Figure 8. Tradeoff between HTSE variability and battery size for two wind profiles

The HTSE variability is found to be much more sensitive to the wind profile than to the battery size. These results show that there remains a very significant amount of variability dictated by the wind that no amount of smoothing from a battery can eliminate, and that the battery can only be useful for this purpose up to a limited extent. Another important result is that accurate modeling of wind for a given site is of critical importance to system design, as the impact of wind profile can significantly exceed those of other design considerations.

IV. CONCLUSIONS AND ONGOING EFFORTS

In this study, we have successfully applied surrogate modeling and analysis tools to study several key aspects of HES performance, including value maximization for multiple competing attributes under varying renewable energy generation conditions and quantification of the relative sensitivity of HES performance to the dynamic properties of three key system components. Battery size calculations show a clear tradeoff between minimizing the variability of electrical power delivered to a load and minimizing the battery storage size. These results are also found to be highly sensitive to the renewable power profile considered, and thus highlight the necessity of properly accounting for variations in wind speed when designing HES that incorporate wind turbines as a renewable resource. A surrogate model is successfully applied to map the global parameter space, and GSA shows a strong sensitivity to the battery time constant.

These sensitivities and their associated uncertainties present an opportunity for adding value to the design of systems requiring a large capital investment and a long operational life, two notable characteristics of HES. When considering an energy system with a long lifespan, designs that are capable of evolving with the changing energy generation landscape may provide significant benefit compared to rigid designs. For example, an HES configuration that can switch between natural gas and nuclear power plants for the baseload generation depending on the relative operating cost can take advantage of periods of low cost for either technology. Real options theory allows for such evolvable designs, and therefore provides a method for reducing the risk attributed to uncertainty in future fuel costs and commodity prices, for example. Our current research efforts include applying real options theory to investigate the viability of evolvable HES designs from the perspective of long-term investments (e.g., 80+ years).

The current HES model uses a series of block diagram models for its subsystems. To more accurately model the true physical phenomena occurring in the system, ongoing research is focused on the development of higher-fidelity physics-based models [17]. Additionally, it is possible to integrate such high-fidelity models into a framework for producing composite or "hybrid" physics-enhanced models such as the one shown in Fig. 9, in which certain physics-based equations are retained while others are simplified using surrogate models. The value in implementing such methods is a significant reduction in the computational cost of performing simulations. By simplifying certain complex phenomena using approximate equations such as a response surface, appropriate detail can be maintained while improving simulation speed. This in turn allows for more in-depth evaluation of the system and its properties.
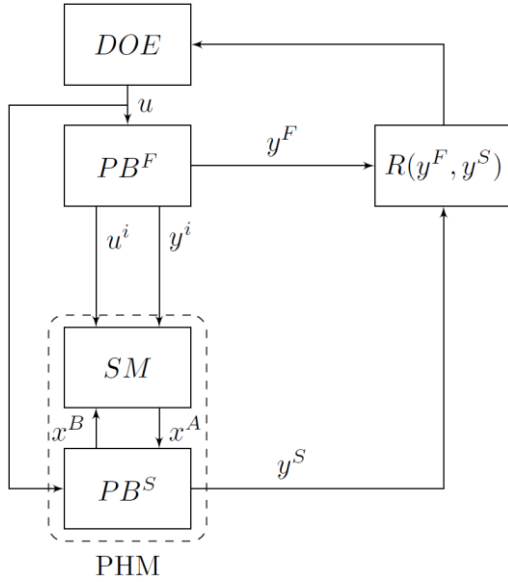
Figure 9. Computational architecture for creating physics-enhanced hybrid models (PHM) that combine physics-based simplifications (PB^S) with surrogate models (SM)

Just like in standard surrogate modeling approaches, a DOE is used in conjunction with a physics-based full-order model (PB^F) to create the physics-enhanced hybrid model (PHM). The difference between the hybrid modeling architecture in Fig. 9 and purely numerical methodologies such as the one illustrated in Fig. 2 is that the level of fidelity can be varied according to the needs of the problem being studied, by assigning only some of the variables of interest to the surrogate model (SM), while others are modeled using physics-based simplifications (PB^S) where the physical equations are retained. Therefore, the PHM can be fine-tuned using the residual calculation R(y^F,y^S) to optimally balance the competing needs of model fidelity and computational efficiency.

As an example from current efforts in this area, this methodology has been applied to create a physics-enhanced model of a boiler in a high-fidelity HES model. The boiler includes a heat exchanger where a phase change can occur in either the tubes or the shell. Due to the large differences in physical properties that occur during a phase change, a large amount of simulation time is dedicated to calculating the precise states at which phase changes occur. A second order response surface model is found to achieve approximately a 50% decrease in simulation time while retaining 99% accuracy, by mapping the flow rates and specific enthalpies at the inlets to the outlet specific enthalpy for the hot side of the heat exchanger. The remaining quantities are calculated using conservation equations.

Finally, other important ongoing research directions include incorporating additional renewable and storage technologies such as concentrated solar and pumped hydro storage into HES models, integration of multiple computational environments within model exchange and co-simulation configurations, and the development of advanced sensing, control strategies, and platforms for the adaptive and optimal operation of HES.

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