Leveraging Digital Twins in the Development of a Novel Solid Oxide Fuel Cell/ Gas Turbine Hybrid System

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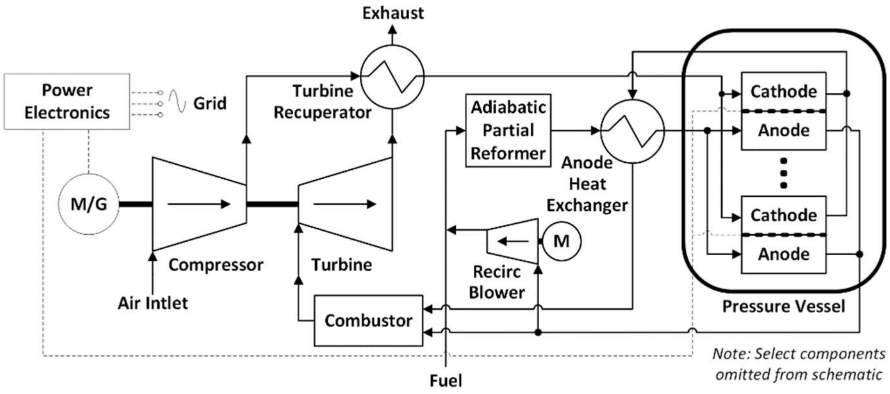
Addressing climate change will require rapidly developing and deploying a myriad of novel technologies. Frequently these technologies are highly complex and effectively transitioning them from lab-scale concepts to real-world applications is an imperative. One technique which is increasingly being leveraged to accelerate clean energy technology development and implementation is known as a ‘digital twin’. In this paper the use of a digital twin to accelerate the development of a Solid Oxide Fuel Cell/ Gas Turbine (SOFC/GT) hybrid system will be explored as case study.

One ‘wedge’ [1] which can be employed to address climate change is to increase the efficiency of energy producers and consumers. Dramatically increasing the conversion efficiency of natural gas to electricity at small-scale distributed locations is the impetus behind the SOFC/GT system currently under development by a team affiliated with the author. This project, with a goal of demonstrating an electrical conversion efficiency of 70% from natural gas (LHV basis) at a 50 kWe scale, is part of the ARPA-E INTEGRATE program. The project is led by Nexceris (NexTech Materials) [2] representing both the PI and developing/supplying advanced planar SOFCs; Czero [3] which is leading the overall system design, controls, construction, and testing; and Brayton Energy [4] leading the turbomachinery development.

A simplified schematic of the SOFC/GT system currently under development by the team is shown below. At its simplest it entails inserting an SOFC within the heat generation portion of a conventional Brayton cycle gas turbine (though the integration of the two systems is much more complex than is alluded to by this simplification). SOFC’s are devices which electrochemically convert fuel into electricity with a high degree of efficiency. One of the more challenging aspects of SOFCs, however, is the requirement to operate at very high temperatures (~750-850C for this specific stack technology). These operating temperatures, nevertheless, are well within typical operating range of a gas turbine.



Note: Select components omitted from schematic

Figure 1: Simplified SOFC/GT System Schematic

The system operates by mixing desulfurized natural gas with recirculated anode tailgas (which contains, among other constituents unconsumed fuel from the SOFC and steam generated by the electrochemical reaction) and passing it through an adiabatic partial reformer. This reformer is a necessary conditioning step which cracks higher hydrocarbons and partially reforms the natural gas stream into a mixture of H_2, CO, CH_4, CO_2, and H_2O though Steam Methane Reforming (SMR) and Water Gas Shift (WGS) reactions which can more readily be consumed by the SOFC. Note a key benefit of SOFC’s is that the temperatures required to reform natural gas are well aligned with the nominal operating conditions of SOFCs. After reheating, the syngas mixture enters the SOFC stack where a portion of the fuel is converted into electricity with O2 ions migrating from the cathode to the anode forming water vapor. System performance is further enhanced by performing a portion of the fuel reforming within the stack itself enabling higher power density and reducing cooling requirements due to the endothermic SMR reaction.

To maximize efficiency within the SOFC, only a portion of the fuel is consumed in each pass through the stack. Much of the fuel is recirculated to the reformer and back through the stacks via the high-temperature recirculation blower. However, to limit the dilution of the fuel mixture within the stacks, a portion of the anode tailgas stream is fed to a specialized combustor within the GT portion of the system. This combustor consumes the remaining chemical energy within the fuel stream (which in a typical SOFC system is vented/wasted) and further lifts the already hot anode/cathode streams which is then fed into the GT's turbine section. The turbine expands this hot gas stream (which would otherwise be wasted in a typical SOFC) and generates shaft power. This shaft power first drives the GT's compressor section which supplies flow to the system, while the remaining power is used to drive a generator. The electricity produced by both the SOFC and the GT generator is controlled and combined within power electronics before being exported to a grid (either in an islanded configuration, or as part of a larger grid).

The compressor supplies a flow of compressed air first to the SOFC and then to the turbine section of the GT. The cathode side of the SOFC requires a high-temperature flow of compressed air as both the oxidant for the electrochemical reaction, and as a coolant to carry away internally generated heat to prevent the stacks from overheating. In a typical SOFC system this heated oxidant stream is supplied by a blower/heater and then vented/wasted (with a recuperator sometimes included to improve efficiency). By integrating the cathode stream into the Brayton cycle this oxidant flow and heat can be effectively and efficiently supplied. Another advantage to locating the SOFC within the hot flow path of the GT is that it allows the SOFC to be pressurized which further increases electrochemical efficiency. By closely integrating the SOFC and GT systems the overall system efficiency can be maximized beyond what either system is capable of in isolation. A rendering of the pressure vessel holding the SOFC stacks at Czero's facility is shown below (the turbomachinery and remaining balance of plant is housed in a second container connected to the open portion of the container shown in this rendering. Note that components of this demonstration system were spread apart to facilitate the development process and would not represent the footprint of a production system).

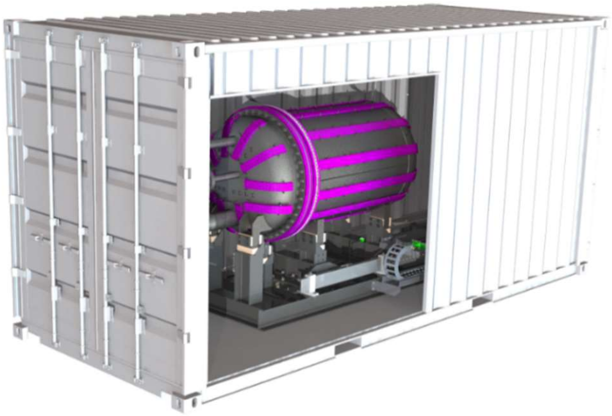


Figure 2: SOFC Pressure Vessel

As described above, the SOFC/GT system is a highly complex and integrated system requiring a substantial effort to rapidly develop and demonstrate this system. This type of development project is highly conducive to the use of digital twins. The term 'digital twin' is broad and has varied connotations in different industries. For this discussion the author is using digital twin to refer primarily to a dynamic plant model of the SOFC/GT system, and to a lesser degree solid models (CAD) of the system.

At its core a digital twin is a virtual representation of a yet-to-be-built or an existing physical system. The digital twin provides predictions on how the physical system will behave under a range of circumstances such as with varied component sizing or control strategies, without incurring the time/expense/risk of evaluating each of these questions on physical hardware. As such the digital twin is more broadly a means to an end in support of a physical system over its lifecycle, rather than an objective in and of itself. To provide value the digital twin must be capable of providing useful predictions of the physical system's response throughout the development and deployment process. At the beginning of a development project the physical system is typically ill-defined, and as such the digital twin constructed to represent this ill-defined physical system will likewise provide only general guidance. However, as the development process continues and becomes more defined, these refinements are iteratively incorporated into the digital twin enabling it to provide more accurate predictions in support of system development. In this way both the system design and digital twin advance in parallel with the digital twin providing information to the system design in support of its advancement, while data from the system design is fed back to the digital twin to improve its fidelity.

As part of the SOFC/GT development process there has been significant interaction between the digital twin and its physical counterpart presently under construction. Several of these key interactions are shown below:

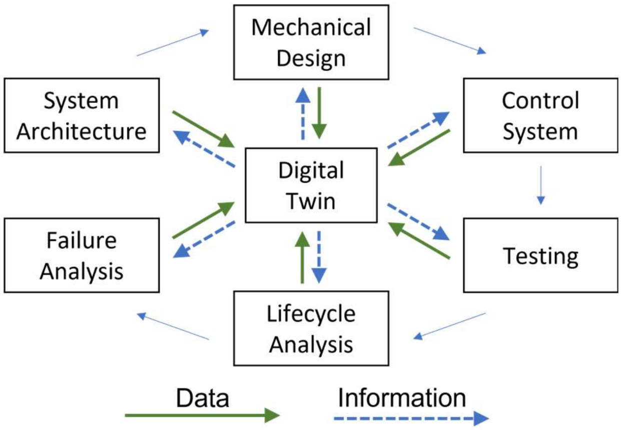


Figure 3: Digital Twin Methodology

The SOFC/GT program started with the development of an initial system architecture (process flow diagram, PFD) which was used as the template to create the first digital twin dynamic model. This dynamic model was vital to the iterative refinement of the system architecture as the model was heavily leveraged to determine the optimal configuration which achieved the required heat/mass balance integration between the SOFC and GT subsystems, while simultaneously maximizing the system's performance and efficiency. Furthermore, the dynamic model was used not only to simulate full load steady-state conditions, but also transients including startup and shutdown. Within these off-design conditions the dynamic model identified areas which required additional components to be added to the schematic to ensure proper system functionality. Throughout the development of the system architecture the PFD was continuously updated based on findings from the digital twin, while the digital twin was simultaneously updated to reflect the most current system architecture.

A key element of the digital twin employed for the SOFC/GT development process was the dynamic system model. The purpose of this model was to accurately predict both the steady-state performance characteristics and transient response of the physical system. It was built in MATLAB Simulink predominantly from governing equations using a custom library developed internally by Czero. It features compressible gas dynamics, real gas properties (from NIST REFPROP [5]) with variable reference conditions and ideal gas extrapolation, individual species tracking (N2, O2, H2O, CO, CO2, H2, CH4, C2H6, C3H8), mixture modeling, electrochemistry for the SOFC, equilibrium chemistry (SMR, WGS) for the reformer and SOFC, rotational dynamics, and turbomachinery based on compressor/turbine maps among other physics. It is predominantly physics based, rather than, for example, a black box model generated based on test data. As such it was able to be generated before any test data was available and can also predict off-design operating characteristics. As more data become available, tunning factors (such as heat transfer coefficients and friction factors) will be adjusted to bring the digital twin model closer to the physical system. The model itself runs relatively quickly, on the order of 10x real time with a variable time step solver, a significant advantage when simulating a system which may take a day to transition from a cold state to fully operational.

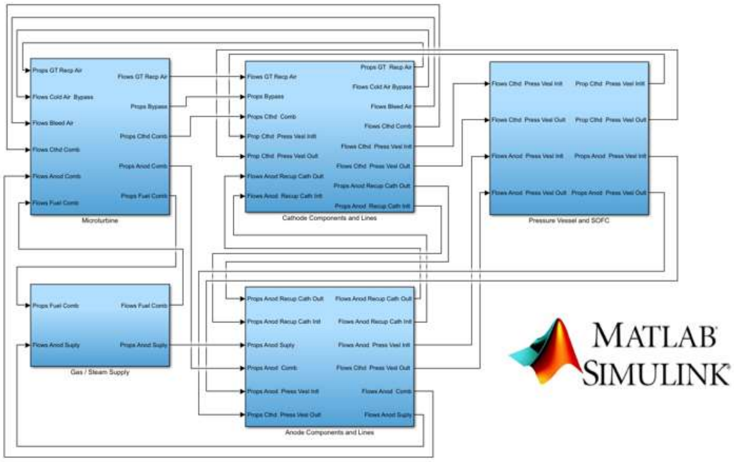


Figure 4: Digital Twin Dynamic Model

Another key element of the digital twin is the CAD or solid model. While a relatively common approach these days, maintaining an accurate solid model of the system as it is being designed not only supports the design/manufacturing process, but also is essential for supporting the system analysis. The digital twin solid model is especially useful for providing accurate inputs to the dynamic system model (such as internal volumes and thermal masses) as well as providing geometry to support structural/thermal FEA and CFD.

Both the dynamic and solid model digital twins were uses extensively as part of the mechanical design process within the SOFC/GT development program. The digital twin solid model was the principal tool used within the design process, while the dynamic model was regularly interrogated to understand how changes in the mechanical design (e.g. line length and size) would influence the physical system's operation. In addition, the solid model digital twin was used extensively to run various types of FEA (Finite

Element Analysis) and CFD (Computational Fluid Dynamics) which were essential given the high temperatures the SOFC/GT system operates at. As these analyses were run, any changes to the system design based on the outcomes of these analysis were then used to update both the dynamic and solid model digital twins. Examples of several types of CFD (top) and FEA (bottom) analysis which leveraged the digital twin solid model as part of the mechanical design process of the SOFC/GT system are shown below:

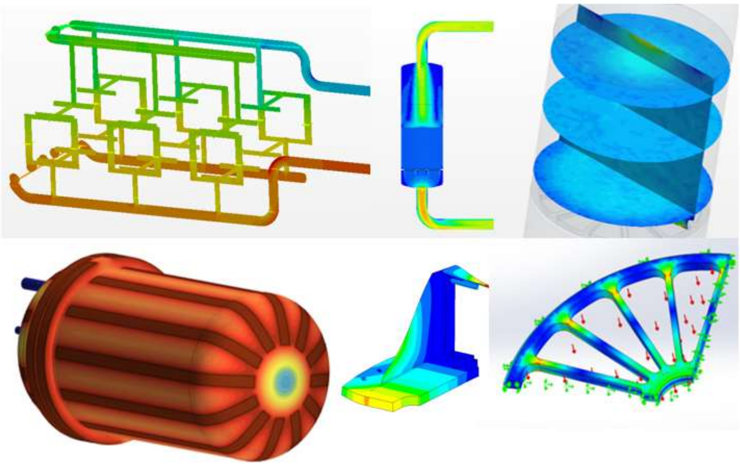


Figure 5: Select CFD and FEA Analysis Leveraging the Digital Twin Solid Model

One of the more complex aspects of the SOFC/GT system is determining how best to control it. This complexity originates not only from the close coupling and narrow band of allowable operating conditions of both the SOFC and GT subsystems, but also with the knowledge that things can go very wrong very quickly with this system. This SOFC/GT system is not conducive to developing/validating control strategies directly on the physical hardware as is common practice with less complex systems. Here again the digital twin dynamic model provides significant benefits in terms of reducing technical risks and accelerating the development timeline.

For the SOFC/GT program the digital twin dynamic model was leveraged first to determine general control strategies. This was done by using an understanding of how this system functions to first implement and evaluate preliminary control strategies, and then refining these control strategies such that the dynamic model responds to the strategies in the manner desired. Examples of the types of control strategies which were identified during this process and implemented in the final controls code include controlling the electrical load placed on the SOFC stacks to achieve the desired stack outlet temperature, operating the GT in speed control mode using power electronics with the reference speed adjusted to achieve the desired turbine inlet temperature, and closing the loop around export power by adjusting fueling. Furthermore, the overall system efficiency predicted by the dynamic model was evaluated over a wide range of reference commands to determine the optimal operating conditions for the SOFC/GT system. Findings from the digital twin dynamic model were used both to the finalize the general control strategies for the control system, and to inform/update the system architecture and mechanical design to ensure the proper control elements, with sufficient range and bandwidth, were in place.

Once the general control strategies were established for the SOFC/GT system, development of the complete controls code began. This controls code is much more complex than the general control strategies as it need to cover startup, shutdown, nominal operation, state transitions, as well as identify and respond appropriately to any faults which may occur. For this program a MATLAB Simulink based controller from Speedgoat [6] was selected. Benefits of this platform include not only a high-performance controller and data acquisition system, but importantly the ability to develop all the controls code in Simulink and then compile and deploy the same code directly onto the controller. This enables most of the controller development and validation process to occur within the same MATLAB Simulink environment which contains the digital twin dynamic model. Throughout the course of the controller development process the controller code was evaluated using Model in the Loop (MIL) methodology. With MIL methodology the controls code is connected to the dynamic plant model and run through its paces using the same sensor inputs and actuator outputs as would be available to the controller in the physical system. This process provides a substantial risk reduction as the controller software is evaluated and validated on the digital twin before ever connecting it to the physical system. Furthermore, this entire controller development process occurred using the digital twin before the physical hardware was built providing a significant reduction in development time. The plot below shows an example of the startup and transitioning to full load using the full controls code running on the dynamic model digital twin:

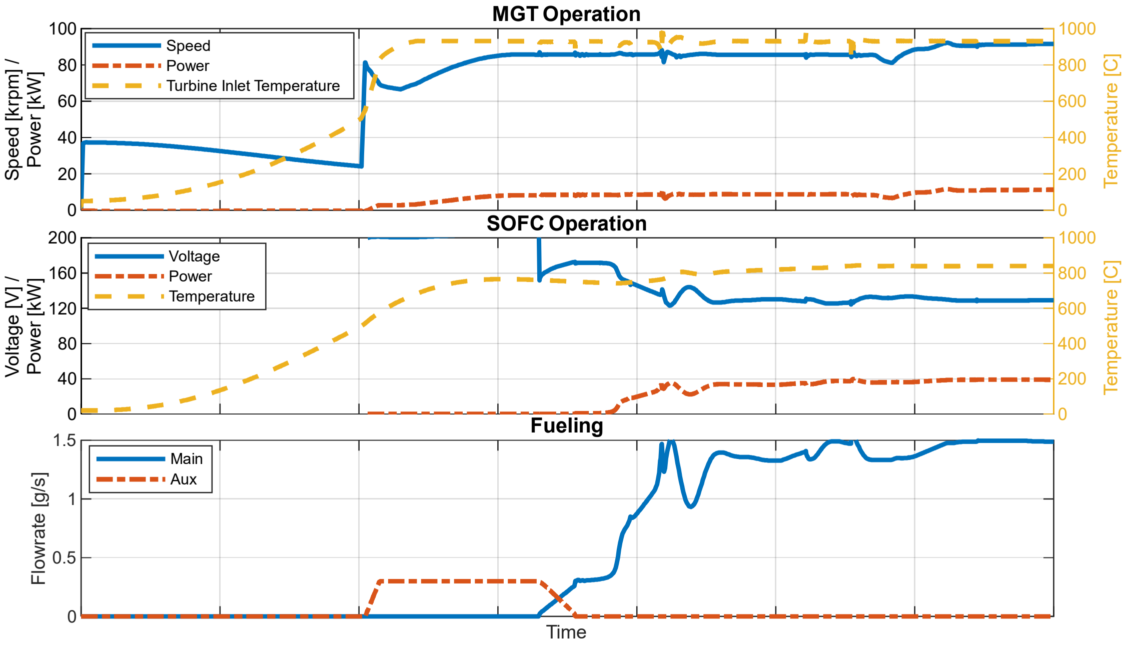


Figure 6: Model in the Loop System Response

In addition to working through the general control strategies as well as startup and shutdown routines, the controls code also had a series of fault detection and response strategies incorporated into it. The benefits offered by the digital twin dynamic model shine here as well. Fault detection and response strategies are essential for a complex system such as this to mitigate risk to personnel and hardware. However, testing these control strategies on the physical system would likely be both inherently hazardous and prone to damaging the system. Rather than, for example, disabling the load on the GT's generator while it is at full speed to evaluate the efficacy of the fault detection and response strategies on the physical system, this same evaluation was conducted using the digital twin with zero risk.

At the time of this papers writing construction of the SOFC/GT system is underway and final preparations are being made for system commissioning and testing. Initial testing of a physical system is typically the point in a project's progression where more confidence is placed on results from the physical hardware than the digital twin (following the adage 'all models are wrong, some are useful'). While *accurate* measurement data should generally be trusted more than model results, digital twins still have an important role during the testing phase. If there are significant disagreements between the digital twin dynamic model and test data from the physical system, then an effort should be made to determine the source of this discrepancy to ensure both the physical system, and digital twin, are functioning as intended. Several potential sources of discrepancy include:

- A component within the physical system may not be functioning as designed
- There may be an issue with sensors/data acquisition which is providing erroneous readings
- The digital twin dynamic model may not accurately represent the physics or parameters of the physical system

Regardless of the sources of this discrepancy, is should be identified to ensure proper system operation. Here again the digital twin dynamic model can provide guidance for troubleshooting these issues by providing predictions for what every state measured on the physical system should be. By comparing the predicted vs measured state points the discrepancy between the two system can generally be identified and addressed. Once confidence is achieved that the physical system is operating as intended, the measurement data is then used to calibrate/validate the digital twin dynamic model to improve the usefulness and predictive capabilities of the digital twin in future development phases.

Once commissioning is complete digital twins may sometimes become relegated to an afterthought, however there are compelling reasons to maintain a robust digital twin. There are multiple instances when a digital twin may be called back into action even if a system is already in production. For example due supply chain or economic reasons a component within the system may need to be replaced with another component possessing somewhat different performance characteristics. In this case it is often best practice to use the digital twin dynamic model to evaluate the influence of changing this component on the system's performance and operability, especially if the original and new component's performance characteristics are significantly different. Another common use case for digital twins in the production phase of a project is to assist with failure analysis. Regardless of how well a physical system is instrumented, invariably not all states of interest related to the failure are recorded (either due to number/expense of desired measurement points, or states which are physically challenging to instrument). Digital twins have the advantage of full state observability which can provide valuable insight into what lead to a failure.

Digital twin dynamic models also have a role to play in advanced control concepts beyond the development and validation efforts already described. The digital twin can be modified such that it can be used as part of model based control strategy to improve the control system performance, especially in cases where highly dynamic interactions and transients are of interest. Furthermore the digital twin model can be used as part of a prognostics and diagnostics strategy to identify and address upcoming failures through preventative maintenance and scheduled downtime to provided additional benefits to the end customer.

While there are numerous benefits for employing digital twins in advanced development programs, there are limitations of the digital twin methodology as well. If the physics behind the system are poorly understood, then the digital twin dynamic model is unlikely to provide an accurate representation of the eventual physical system. Likewise the digital twin dynamic model is only capable of identifying potential issues with the physics which are included within the model. In the case of SOFC/GT system several issues with material corrosion were identified during furnace testing of the materials which were not detected by the digital twin (as material corrosion was not included within the digital twin physics). Care must be taken to remember that the digital twin methodology is a tool with its own limitations and does not replace proper engineering rigor.

This paper describes digital twin methodology employed to accelerate the development of a unique Solid Oxide Fuel Cell/ Gas Turbine hybrid system. Digital twin methodology will enable the project team to go from a rough concept to a fully-functional technology demonstrator within an anticipated 2.5 year timeframe. Both dynamic and solid model digital twins have already demonstrated their worth multiple times over during this highly complex development project. These methodologies are almost certain to provide significant benefits in terms of accelerating and de-risking future clean energy development programs in the years to come.

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