Advanced MATLAB/Simulink Multi-Species/Multi-Phase Block Set

Introduction

Czero has developed custom MATLAB/Simulink library block sets for simulating an array of systems that include mechanical, fluid, chemical and electrical processes. The block sets were developed in response to the need to have detailed modeling of fuel cells, electrosynthesizers, chemical storage reactors, gas turbines, and other systems for our customers. Different blocks can be combined to build up multi-domain models of varying size and complexity. This paper focuses on block sets developed within the Simulink environment which model multiple species and two-phase fluids integrated with chemical reactions and heat transfer. This paper also describes the physics and implementation of specific blocks using examples of both a gas turbine Hardware-in-the-Loop (HIL) system, and a Solid Oxide Fuel Cell (SOFC) gas turbine combined system under development at Czero.

Modeling and Simulation

Modeling and Simulation (M&S) are an integral part of system and controls design in modern engineering. M&S tools allow engineers and designers to create virtual representations of systems, products, or processes and analyze their behavior under various conditions. Some of the key benefits are:

- Cost and timeline reduction
- Parameter sweeps and optimizations
- Visualization of complex systems
- The ability to perform Model-in-the-Loop (MIL), Software-in-the-Loop (SIL), and Hardware-in-the-Loop (HIL) testing
- Evaluate abnormal conditions that might otherwise damage hardware

Czero works on a vast array of technologies, many of them novel and which combine multiple physical domains. For example, models of fuel cell systems will combine mechanical elements (actuators, compressors, blowers, valves), fluids (gas, liquid, or both), chemical reactions, heat transfer, and electrical power flow. In many instances, the system model needs to simulate all the major components to effectively:

- Predict the system's performance and transient behavior
- Size system components
- Develop a control system

As computer processing capabilities improve, more complex systems can be modeled with M&S tools. MathWorks's MATLAB/Simulink is a powerful, widely used M&S tool that is frequently the software package of choice for Czero engineers developing models. It is particularly useful in the field of dynamic modeling, control system design and tuning, and signal processing. Simulink models have numerous benefits:

- Intuitive block diagram interface
- Multi-domain modeling
- Openness and extensibility
- Model-based design for systems
- Parameter sweeping and sensitivity analysis
- Real-time simulation for MIL, SIL, HIL

Over the years, Czero has developed a library of custom blocks within Simulink. This library is combined with internally developed customer specific blocks for efficient development of M&S tools, which are then leveraged for all the reasons discussed above. This workflow is captured in Figure 1. This paper will discuss some of these blocks, including example fundamental and subsystem blocks within the standard library, in addition to a gas turbine HIL system and fully integrated SOFC gas turbine combined cycle system model. These block sets were created out of the necessity to model more complex systems while maintaining reasonable run times so that large parameter spaces could be explored. Furthermore, reasonably fast simulation run times are highly preferred for MIL/SIL testing, and critical for real-time HIL testing, when developing control systems.

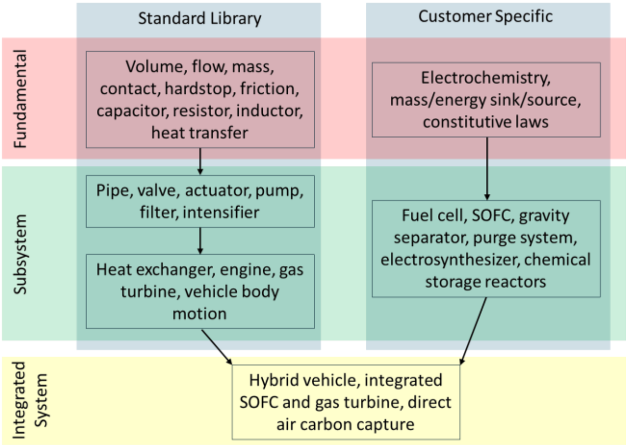

Figure 1: M&S library workflow

Czero Fundamental Block Set

This section highlights fundamental blocks developed by Czero for use in the development of M&S tools. Specifically, this section discusses the more commonly used fundamental thermodynamic/fluidic blocks and provides a high-level description of how chemical reaction blocks are developed.

Fundamental Thermodynamic/Fluidic Blocks

For thermodynamic/fluidic system, volume and flow elements are the two most common fundamental blocks. Details of these blocks vary by application, such as whether it is liquid or gas, compressible or incompressible, ideal or real gas properties, and the level of fidelity required. Additionally, these blocks have been adapted over the years to handle scenarios where multiple species and multiple phases exist, a common occurrence in the types of complex systems discussed throughout this paper. Additional content related to multiple species and multiple phases is provided later in this section.

- The volume element evaluates pressure, temperature, and other fluid properties subject to the flows in and out of that block. Both mass and energy are conserved as shown in Figure 2.
- Conversely, the flow element evaluates mass and energy flow rates subject to adjacent pressure, temperature, and other fluid properties. Momentum is conserved as shown in Figure 3.
- Causality is fixed and can easily be integrated and combined with other fundamental blocks or subsystems.
- Depending on the application, thermodynamic and transport properties are extracted from REFPROP, the Standard Reference Data program of NIST (Lemmon et al. 2010), using computationally efficient means.

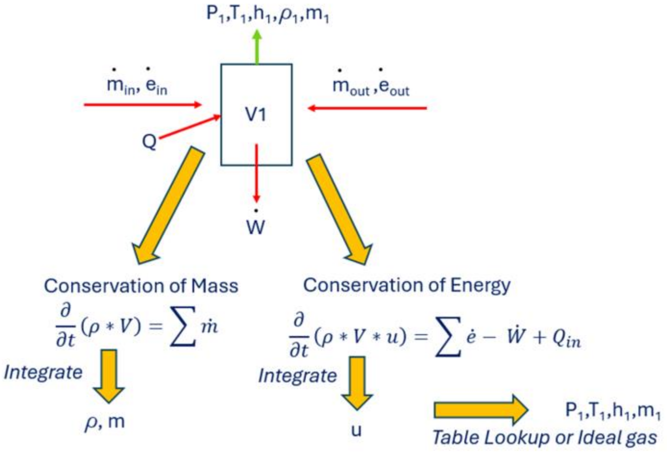

Figure 2: Volume block physics

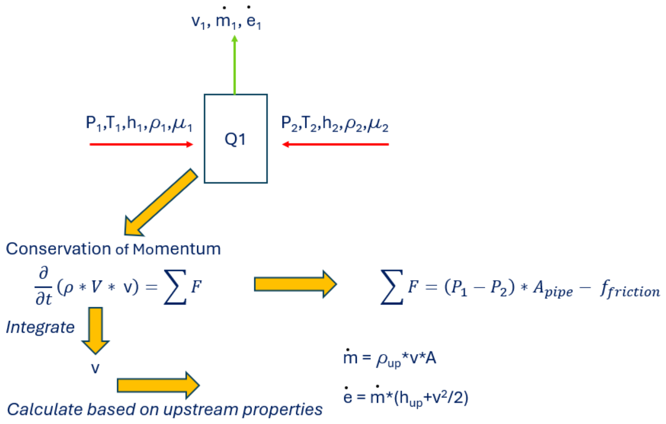

Figure 3: Flow element block physics

The inclusion of multiple species is necessary when considering processes involving chemical reactions, such as in fuel cells, engines, and carbon capture systems. Implementing multiple species presented a unique set of challenges.

- Both total and individual species mass and total energy and momentum must be conserved. This requires extensive bookkeeping and is accomplished using vector mathematics on vector signals.
- Additional challenges include the complexity of evaluating mixture properties while being computationally efficient. While REFPROP can provide these mixture properties, it is not practical to do so in a simulation environment. Instead, a reduced set of REFPROP data is generated *a priori* and combined using mixtures models to obtain the requisite thermodynamic and transport properties.
- The result is a model that incorporates accurate thermodynamic and transport properties yet is computationally efficient.

Similarly, the inclusion of multiple phases is also necessary and presented a unique set of challenges.

- These blocks utilize similar bookkeeping and vector strategies as the previously developed multiple species blocks. However, they are further discretized to include both liquid and gas phases.
- Phase change of a species is allowed within a volume block and calculated from the conditions of that same volume.
- A custom internal Newton-Raphson numerical solver is used to identify the quality of the condensable species subject to the same mass and energy conservation constraints, in addition to the saturation properties of the condensable species.
- To improve computational efficiency, these saturation properties are obtained from multivariable curve fits generated *a priori* using limited REFPROP data. For convenience, this process is automated based on user specified species and bounds on operating conditions.
- As with previous blocks, thermodynamic and transport properties are incorporated using REFPROP data and mixture models. Additional models are required for two-phase mixing and transport properties.
- The thermodynamic and transport properties are used by other multiple phase thermodynamic/fluidic blocks, such as line, orifice, and heat transfer blocks.
- Depending on the application, additional blocks are developed that may sink or source mass and energy based on current phase separation and known physics and/or data. For example, Czero has developed physics-based blocks for liquid/gas gravity separators, membrane humidifiers, electrosynthesizers, and more.

Fundamental Chemical Reaction Blocks

Czero frequently develops chemical reaction blocks based on the physics of interest for a particular client and application. Some recent applications include electrochemistry within SOFC and PEM fuel cells, the steam methane reforming process, combustion processes, and various types of carbon capture chemistry. Typically, these blocks act as energy and mass sinks and sources based on the underlying chemistry defined by physics or data-based correlations. The correlations are often developed independently by Czero or in collaboration with the client.

The chemical reaction blocks will determine the product and reactant species stoichiometry as well as how much of the reaction occurs. The reaction blocks can be rate based or assume thermal equilibrium chemistry. For thermal equilibrium chemistry, internal

Newton-Raphson solvers are implemented to determine the species' equilibrium mole fractions within the volume.

Based on the change of species that occurs, and the heat of reaction for the given process, the heat added/removed from the volume is calculated. The calculated energy and mass source/sinks are then combined with the flow streams in the volume block to calculate new volume fluid properties. In most cases, the mass species sink results in a mass source of different species in the same or adjacent blocks. During these reactions, mass and energy are conserved. However, the species present do change based on the reaction chemistry. In addition, the heat of reaction is added as a heat source term to the volume, or adjacent thermal mass as is the case in fuel cells.

Example Subsystems Models

Many models are the connection of multiple fundamental blocks or subsystems. A pipe model, for example, may consist of an arbitrary number of volume and flow elements connected to form a 1D system of arbitrary fidelity and computational complexity. Such a system is shown in Figure 4. Here, volume and flow elements are fundamental blocks. This section provides insight into three subsystems, each of which is used within the gas turbine HIL model and SOFC gas turbine combined cycle example later in this paper.

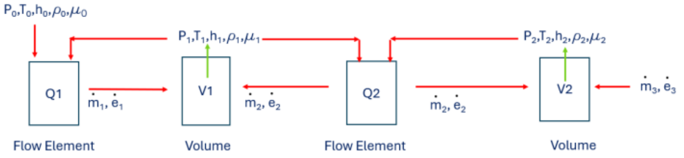

Figure 4: Pipe element created from volume and flow elements

Heat Exchanger

A heat exchanger is a device that allows for the transfer of heat between two fluid streams. Such a device can be modeled using the fundamental blocks discussed previously, such as the volume and line elements, in addition to fundamental thermal mass, conduction, convection, and radiation blocks. This provides the flexibility of having entirely unique fluid streams with unique assumptions (multi-species, multi-phase, real gas, liquid, etc.). These blocks can be connected in arbitrary ways to form any arrangement, and with any level of discretization, both along an axis of flow and in the direction of heat transfer. A typical heat exchanger model is shown in Figure 5, where orange and green blocks are fundamental volume and line elements, respectively, modeling the physics of two fluid streams. This model also includes a central heat exchange block which includes thermal mass of the wall, heat transfer to and from each fluid, and convective and radiative heat transfer to ambient.

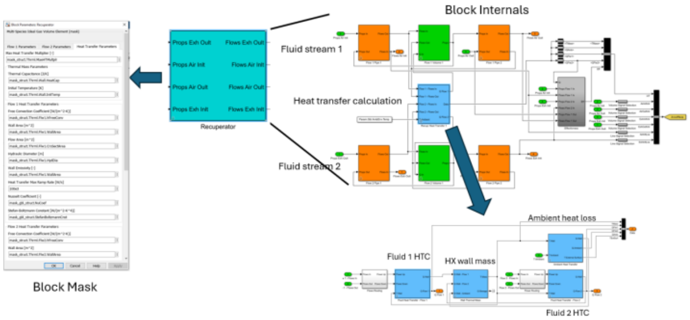

Figure 5: Heat exchanger block internals

Solid Oxide Fuel Cell

A solid oxide fuel cell (SOFC) is an electrochemical device that generates electricity by oxidizing a fuel. An example block is shown in Figure 6. The SOFC operates via electrochemical reaction and heat transfer between two fluid streams, the fuel and air channels. As such, it can be modeled using the previously discussed fundamental blocks in addition to custom electrochemistry and heat transfer blocks.

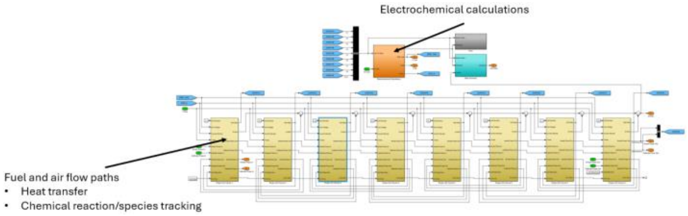

Figure 6: SOFC block internals

The block consists of three coupled subsystems:

- Electrochemistry at anode – electrolyte - cathode interface
- Fuel and air flow channels
- Thermal masses separating channels

The cell is discretized in the direction of fuel and air flow to account for:

- Changes in species as fuel is consumed
- Temperature changes
- Current density variations in the cell due to the previous two variables

The outputs from this model are:

- Cell voltage
- Fuel consumption
- Fuel and air stream temperatures
- Species at each location along the fuel cell channel path
- Heat release

This custom electrochemistry block incorporates the physics for this specific customer's fuel cell chemistry. Cell potential and voltage are calculated using a custom solver with fuel and air partial pressures, which are calculated in the discretized multi-species volume elements that model the fluid streams. These physics are coupled in that the discretized cell current and voltage ultimately drives changes in the thermodynamic properties and heat transfer of each stream, and thus the partial pressures of each stream.

Gas Turbine

A gas turbine (GT) is a system that uses expansion of a continuous flow to produce rotational power. That rotational power can then be used to drive a generator, vehicle, propeller, etc. In this example, air enters the GT and is compressed and pre-heated with the exhaust gas in a recuperator. Fuel is then added to the compressed air stream and combusted in the combustor. The exhaust gas is then expanded in the turbine and goes to the recuperator where it preheats the combustion air before exiting the turbine. The outputs from this model are the GT shaft speed and torque as well as flow rate, pressures, and temperatures throughout the GT.

An example gas turbine block is shown in Figure 7. The block consists of four subsystems connected by multi-species volumes:

- Compressor
- Recuperator
- Combustor
- Turbine

The compressor and turbine consist of inlet and outlet volumes. The mass and energy flow between these volumes are determined using compressor maps, which determine flow as a function of the inlet and outlet thermodynamic properties and shaft speed. The recuperator is like the heat exchanger discussed above, including thermal mass and heat transfer between fluid streams. The combustor uses fuel and air inputs to calculate heat release and required species' sinks and sources.

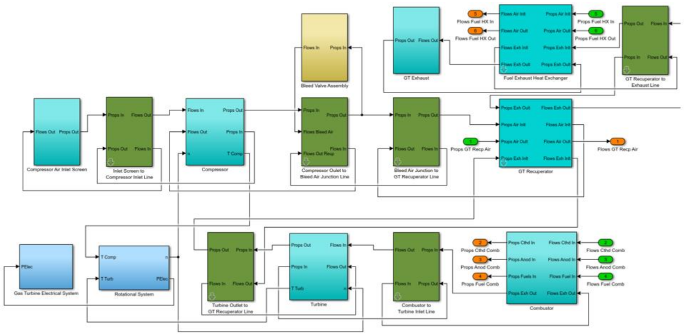

Figure 7: Gas turbine block internals

Example Application: Gas Turbine Hardware-in-the-Loop System

Czero recently completed a modeling and simulation driven project utilizing a version of the multi-species real gas block set to model the AGT-1500 gas turbine and drivetrain in the US Army's Abrams platform. This model was deployed by Czero as part of a HIL simulator for use in the development of a new controls system (Sprengel et al. 2020). Czero leveraged the previously described real gas block set to quickly and effectively create a high-fidelity model that was tuned/validated against multiple sets of measurement data. Figure 8shows an open-loop control response comparison of the HIL model verses measured dyno data, as well as an example of model causality.

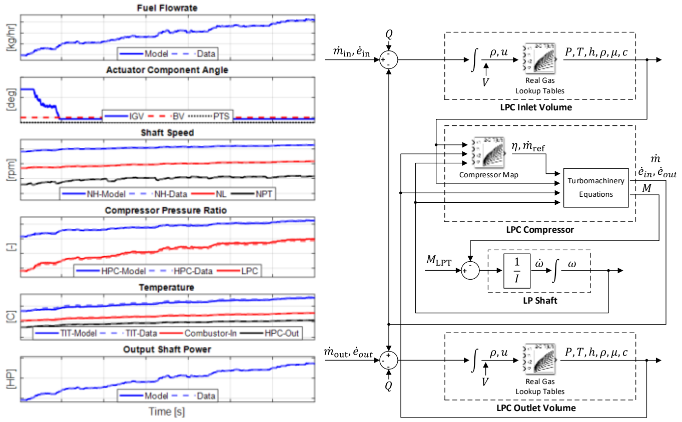

Figure 8: HIL model versus measured dyno data (left), example model causality (right)

Once validated on a PC, the model was deployed on a high-performance LABCAR HIL system and connected to the controls hardware/software under development via a standard wiring harness. Is this way the control system was 'spoofed' into believing it was connected to the actual powertrain, when it was actually connected to the HIL simulator. This simulator took in actuator commands from the controller, simulated how the system would respond using the physics-based plant model, and mimicked appropriate sensor output values. On the LABCAR hardware, Czero's real gas block set allowed the HIL model to run with a 1.3 ms time step using a 4th order Runge Kutta solver, a rate appropriate for the controller under development. Figure 9 shows the overall setup of the LABCAR HIL system.

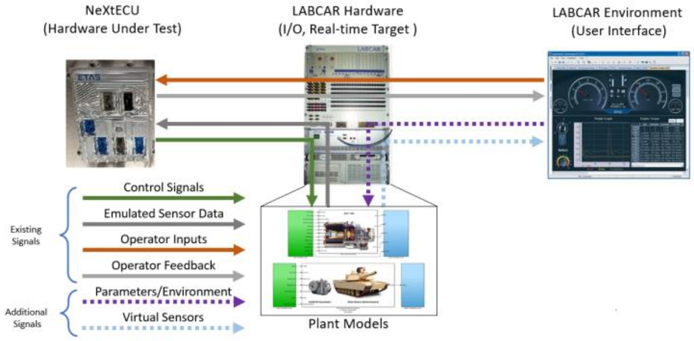

Figure 9: LABCAR HIL system layout

Example Application: Solid Oxide Fuel Cell Gas Turbine Hybrid System

Czero is part of an ARPA-E INTEGRATE (DE-AR0000956) project team designing, building, and testing a combined power generation cycle consisting of an integrated SOFC/GT hybrid system with the objective of demonstrating >70% fuel to electrical conversion efficiency. Project partners include Nexceris as the prime contractor and SOFC developer, Brayton Energy designing a custom gas turbine for this application, while Czero led the overall system design, analysis, controls development, fabrication, and testing at our facility. The SOFC/GT system located at Czero is shown in Figure 10 below. More information on this project can be found in Sprengel 2022, and Sprengel and Echter 2024.

Figure 10: SOFC pressure vessel and BOP in test cell (left), SOFC/GT supporting equipment (right)

A schematic of the system is shown in Figure 11. The system consists of an SOFC, as described earlier, where air and reformed natural gas are combined to produce electricity. Efficiency is increased beyond a standard SOFC by including a GT that combusts the remaining fuel in the SOFC exhaust, which in turn generates additional electricity and boosts the SOFC air inlet pressure for added electrochemical efficiency. A reformer and anode fuel recirculation system are also included to convert the natural gas supplied to the system into hydrogen which can be consumed by the SOFC. The reformer converts the supplied natural gas and recirculated anode tail gas between CH4, CO, CO2, H2O, and H2 utilizing steam methane reforming and water gas shift reactions. These reactions are implemented in the Simulink model using thermal equilibrium equations and an embedded solver. To function efficiently and safely, each subsystem must work in coordination. Modeling these subsystems requires use of all the blocks previously discussed.

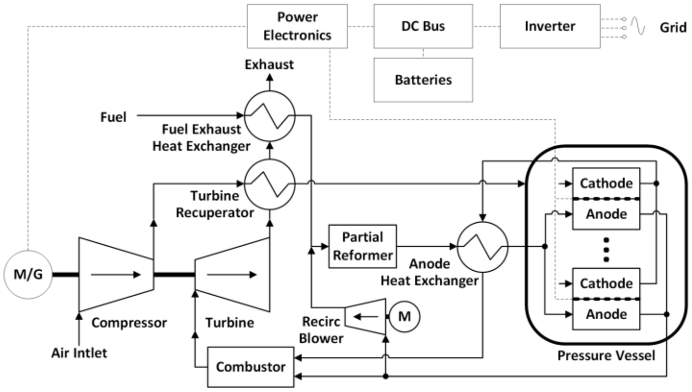

Figure 11: SOFC gas turbine combined cycle schematic

The system is highly complex, sensitive to operating conditions and control, prone to failure if controlled improperly, operates at high temperatures (850 C in the SOFC, 930 C in the GT), and utilizes potentially hazardous fuels. It would have been costly, inefficient, and risky to design and build this system without utilizing extensive M&S for both the system design and controls development.

The system model was utilized for:

- Architecture development
- System and component sizing
- Performance predictions
- Boundary conditions for structural and CFD analyses of the SOFC pressure vessel
- Control system development and validation

For this application, a version of Czero's custom block set was utilized which included only the gas phase (due to the elevated temperatures throughout the system) as well as tracking of nine individual species (N_2, O_2, H_2O, CO, CO_2, H_2, CH_4, C_2H_6, and C_3H_8). To aid in computational efficiency, each control volume was pre-assigned a reference temperature/pressure. During the initialization process, the thermodynamic and transport properties for all the gas species were stored at that reference temperature. During simulation, ideal gas approximations were used to extrapolate the individual species properties based on the difference between actual and reference conditions, which were then combined using various mixing models. This contrasts with the previously described gas turbine model which utilized real gas property lookup tables, but which only included two 'species', air and H_2O.

MALTAB/Simulink was used not only for system analysis, but also for controlling the integrated system. All Supervisory Control and Data Acquisition (SCADA) functions were implemented in MATLAB/Simulink and deployed on a high-performance Speedgoat real-time target (Figure 12). Before deploying the controls code on the physical hardware, it was validated using a MIL approach where the controls code was connected to the previously developed dynamic plant model and heavily exercised. In this case, MIL rather than HIL validation was performed in part because it allowed the testing to be performed faster than real-time (averaging ~100x faster than real-time with 850 states) which would have otherwise been required with a HIL setup. This was highly advantageous for this system as some of the control sequences tested had a duration of multiple days and testing these using a real-time HIL would have been cumbersome and hindered rapid iteration.

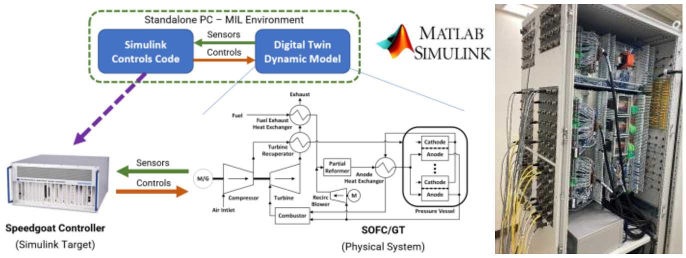

Figure 12: control system MIL approach (left), Speedgoat SCADA system (right)

Conclusion

Dynamic system modeling and simulation techniques provide significant advantages when developing novel and complex technologies. Select advantages include the ability to advance the pace of technology development, optimize system performance and reduce technical and programmatic risks to name just a few. To better support our clients with these efforts, Czero has developed a custom library of advanced multi-species multi-phase blocks in MATLAB/Simulink. This white paper has briefly covered this block set and provided several examples of how this block set has been successfully used on several client projects.

Select Prior Projects

Czero has utilized versions of the multi-species multi-phase real gas block set of a wide range of applications, prior example projects include:

- Direct and point source carbon capture
- High pressure H2 compression
- PEM fuel cells
- Solid oxide fuel cell/gas turbine hybrid system
- Alkaline electrolyzer
- Gas turbines
- Refrigeration and heat pump systems
- Waste heat recovery systems
- High-temperature thermochemical energy storage

How Czero Can Help You

Czero's focus is on helping innovative companies solve the toughest engineering problems through deep expertise, creative thinking, and sophisticated analysis tools. Turn your ideas and design concepts into reality with the help of our product development expertise.

Company Profile

Czero, Inc., founded in 2007 in Fort Collins, CO, is an engineering services company specializing in developing new products and systems with a focus on design and technology advancement for energy conversion, use, and storage.

Czero's core business is working with global clients to create ideas and designs for energy generation, storage, and conversion, focused on delivering more efficient, longer lasting, lower cost solutions.

Concept-to-prototype engineering R&D

Specializing in early-stage R&D and product development Czero uses sophisticated design, analysis, controls, and algorithm development skills to solve tough problems, transforming early-stage concepts into robust proof of concept prototype systems that can be tested to demonstrate commercial viability.

Services

- Dynamic systems modeling and simulation (Czero is a MathWorks Partner)
- Finite element analysis (FEA) and computational fluid dynamics (CFD)
- Embedded controls
- Mechanical design and solid modeling
- Fabrication, prototyping, and testing
- Program and project management

R&D Specialties

- Energy conversion, efficiency, and recovery
- Algorithm and control system development
- Advanced machine design
- High-temperature systems (e.g. 500-1500 C)
- Thermodynamics and chemical processes
- Balance-of-plant development
- Mechanical, electromechanical, and electrohydraulic systems
- High-bandwidth hydraulics
- Automotive powertrains
- Fuel injectors
- Hybrid vehicles

References

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