WHITE PAPER

Designing Fuel Cell Systems Using System-Level Design

Modeling and simulation in Simulink and Simscape

This white paper describes the use of Simulink® and Simscape™ to design and simulate a fuel cell system for electric mobility. It will show by example how Simulink and Simscape support:

- Multidomain physical modeling and simulations of fuel cell systems including thermal, gas, and liquid systems.
- Different levels of modeling fidelities.

MathWorks®

For decades, fuel cells have been used to power various applications. An example is the use of fuel cells in the US space program. Today, hydrogen-powered fuel cells are considered one of the building blocks of a green mobility transformation.

Although their long-standing use implies a proven, mature technology, deploying fuel cells as power sources for electrical mobility poses several challenges, such as effects on vehicle efficiency and range.

A fuel cell electric vehicle (FCEV) drive system consists of many components from different engineering domains including electrical, control, mechanical, thermodynamics, and even chemical to manage diffusion of gases through the fuel cell membrane. The design of these components individually and as a whole system will affect the performance of the vehicle. Modeling and optimizing your designs will help you test a wider range of conditions, shorten development times, and reduce costs.

This white paper describes the design and parameterization of a fuel cell model and its supporting systems (the balance-of-plant) using Simscape. The model makes use of a custom membrane electrode assembly (MEA) block `FuelCell.ssc` supplied with Simscape Fluids™ as well as a custom multispecies gas domain specifically designed for fuel cell modeling.

It is based on a Polymer Electrolyte Membrane (PEM) fuel cell, which is the most popular type of fuel cell for mobility applications due to its low operating temperature, low pressure, and high efficiency. The model also contains the balance-of-plant components.

Why Use Fuel Cell Models?

Using fuel cell models instead of traditional hardware prototypes has numerous benefits spanning across design stages. You can compare design variants, perform tradeoff studies, and select and size components to achieve the desired performance. Once an initial model is created, you can optimize parameters and identify the best operation strategies.

Fuel Cell Model Uses

Fuel cell models are used in many ways, including to:

- Select and size components
    - Perform tradeoff studies using different design variants
    - Optimize parameters and operation strategies
- Design and validate control algorithms
    - Manage thermal and humidity
    - Control pressure
- Analyze performance
    - Analyze energy flows between batteries and fuel cells
    - Determine FCEV range using driving profiles

The benefits of simulation include:

- Shorter development times
- Wider range of tested conditions
- Reduced cost of testing

Such models also enable you to design and validate control algorithms and logic along with the system even before hardware is available. You can start from a simplified model and mature your control strategies together with the overall system.

When the system design is complete and validated, you can implement the components using code generation. MATLAB®, Simulink, and Stateflow offer capabilities for C/C++, HDL, and structured text code generation that can run on any processor, FPGA, or PLC. Specifically for automotive applications, code generation features also include support for AUTOSAR-compliant workflows.

Using simulation models lets you explore a wider range of fuel cell operating conditions, including those that may not be practical or safe when using hardware prototypes. You can also analyze the overall performance of the fuel cell system, such as determining energy flows between batteries and fuel cell stacks and estimating FCEV ranges. The insight gained from simulation helps you develop better hardware prototypes, thereby improving the effectiveness and reducing the cost of testing.

Defining the Fuel Cell Model

Simscape models capture the behavior of complete fuel cell systems down to detailed thermodynamic and diffusion characteristics of mixed gases as well as in the thermo-liquid domain for temperature management and humidification.

The model below (Figure 1) uses a custom library and a custom Simscape domain for multispecies gas modeling. The membrane electrode assembly is a custom component designed using Simscape code that you can adapt to meet specific requirements.

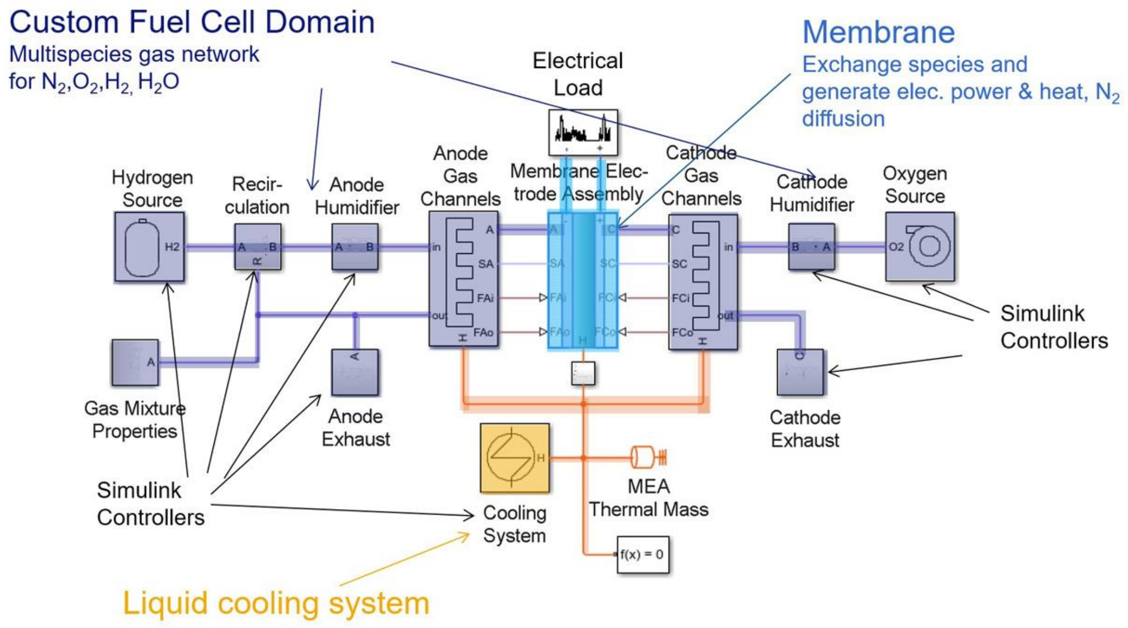


Figure 1. Fuel cell system using the custom fuel cell domain including membrane model.

For more information, please see this example: [PEM Fuel Cell System.]

Sections highlighted in light purple represent the custom fuel cell domain. It addresses the special complexities of fuel cell systems that arise because they are multispecies gas networks. The thermodynamics and fluid characteristics of a mixture of four different gaseous species need to be considered: nitrogen (N_2), oxygen (O_2), hydrogen (H_2), and water (H_2O).

The membrane, highlighted in blue, is written in the Simscape language, which will be briefly covered towards the end of this paper. The membrane model calculates electrical behavior using Faraday's law, the Nernst equation, and the membrane's connection to the electrical load powered by the cell stack. Its properties also account for the diffusion of nitrogen, a critical capability for the design of purging strategies, which in turn are required to optimize efficiency and power output and determine the required battery size.

The orange color denotes the thermal management system. The fuel cell stack needs to be operated at around 80 °C and produces waste heat, so thermal management using coolers, heat exchangers, pumps, and heaters for a cold start are required for the balance-of-plant.

Many of the components of the fuel cell system require different types of controllers, as indicated in Figure 1.

Fuel Cell Model Components

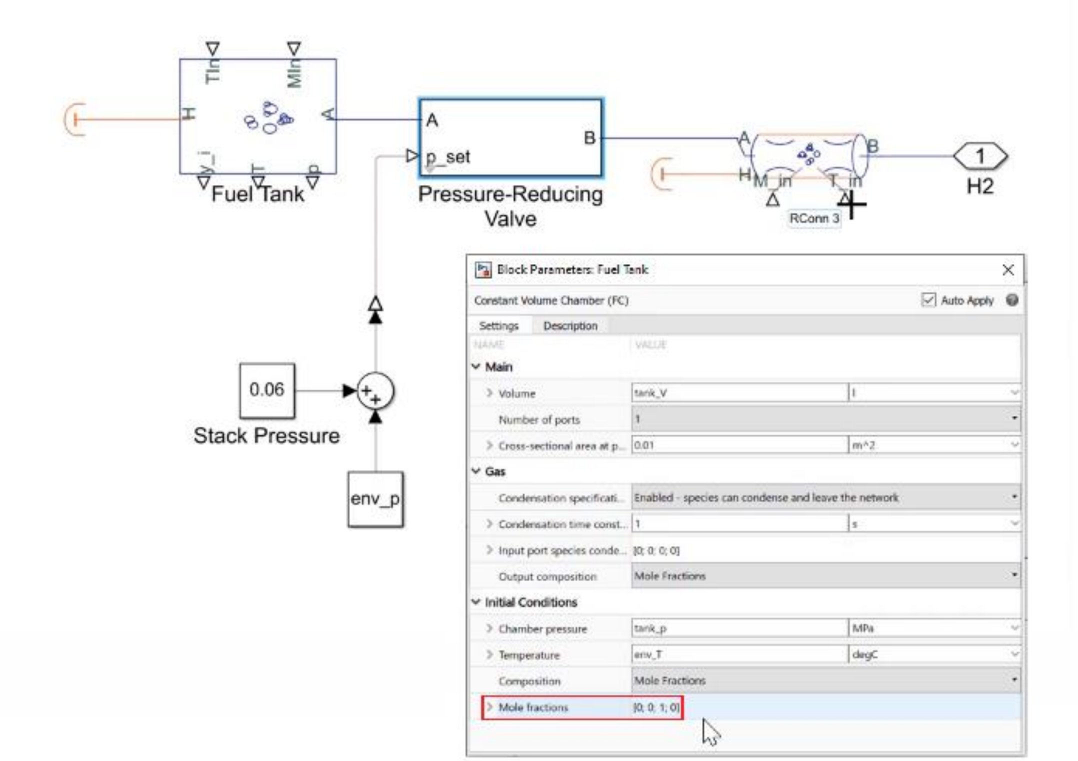
Simscape offers options for modeling fuel cells at different fidelity levels. A later section covers selecting an appropriate fidelity level. Individual components from different engineering domains can be accurately modeled together with their controllers.

The basic components of the fuel cell include:

- hydrogen source
- recirculation system
- humidifier
- anode
- exhaust and purge system

Hydrogen Source

The hydrogen source consists of the fuel tank, a pressure-reducing valve, and a pipe (Figure 2). The tank constitutes a constant volume chamber, a concept used throughout the model. Figure 2 also shows the parameter list for the tank block. Since only hydrogen is stored in the tank, the initial mole fraction (red box) covering all four species is set to one only for the third species, hydrogen. The fixed order of species are nitrogen, oxygen, hydrogen, and water. We will keep finding that vector throughout the modeling process.



Block Parameters: Fuel Tank

Constant Volume Chamber (FC)

NAME	VALUE	
Main		
Volume	tank_V	l
Number of ports	1	
Cross-sectional area at p...	0.01	m^2
Gas		
Condensation specificati...	Enabled - species can condense and leave the network	
Condensation time const...	1	s
Input port species conde...	[0; 0; 0; 0]	
Output composition	Mole Fractions	
Initial Conditions		
Chamber pressure	tank_p	MPa
Temperature	env_T	degC
Composition	Mole Fractions	
Mole fractions	[0; 0; 1; 0]	

Figure 2. Tank with pressure reducing valve and controller.

The tank receives external mass flow (MIn) at a certain temperature (TIn). It has a thermal connection port (H, left) which in this case is insulated and a port (A) connecting it to the next unit, the pressure reducing valve. The tank also has measurement outputs for pressure (p), temperature (T) and also the mole fractions (y_i) of all the four species covered. The attached valve reduces the hydrogen pressure of the tank, which is about 700 bars, to the 1.6 bars required for the fuel cell stack. The valve’s port B is attached to a pipe element that has mass flow (MIn) and temperature (TIn) inputs and a thermal port, which are not used here.

Recirculation

Recirculation (Figure 3) is modeled because not all hydrogen is used in the anode. Unused hydrogen is recirculated instead of being exhausted to the environment. The recirculation element is a constant volume chamber with three ports. Attached to port B is an injector with a controller that controls flow from (R) to port (B) of the volume chamber depending on the current used by the electrical load on the stack (i_stack, bottom left).

The recirculation model enables you to see the impact on efficiency of changing the ratio of fresh hydrogen and used gas reflowing from the anode.

In a later section, simulation using Simulink and Simscape will help validate the design and controllers. You can explore the design space thoroughly before prototyping a system using hardware.

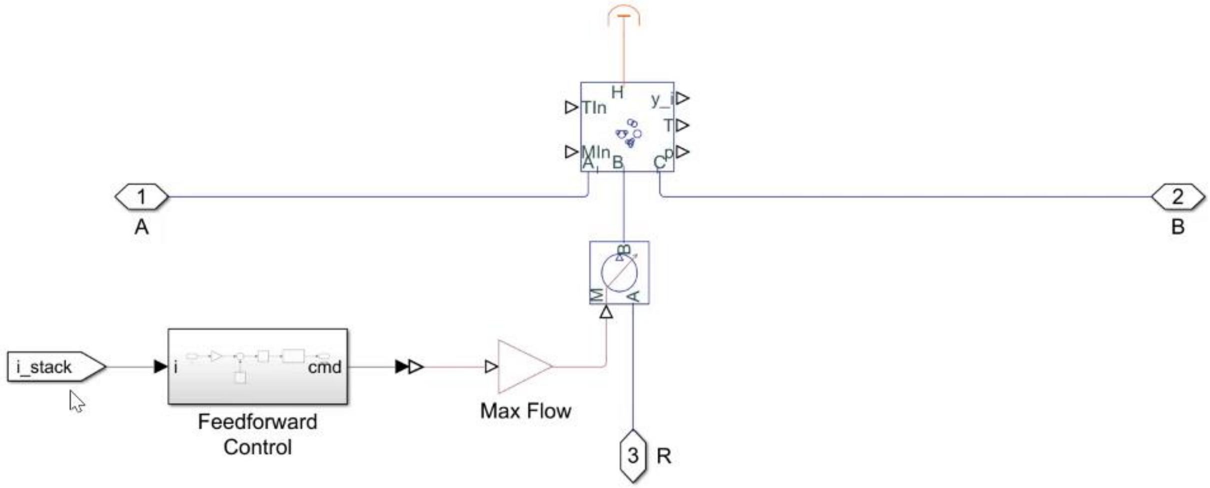


Figure 3. Recirculation with controller and valve.

Humidifier

The anode humidifier attaches to port (B) of the recirculation system (Figure 4). The membrane needs to be kept moist during operation or will otherwise be damaged. To achieve this, the humidifier keeps the relative humidity of the gas mixture entering the anode at 100 percent by injecting water vapor to the pipe over M_in.

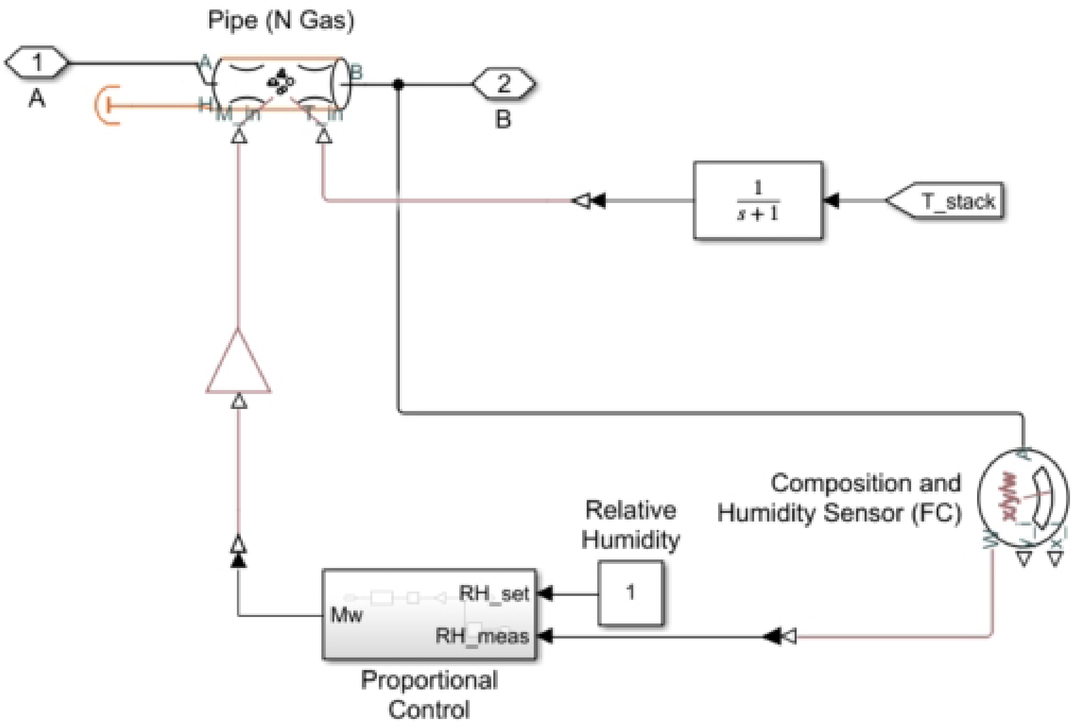


Figure 4. Humidifier element including composition and humidity sensor at the membrane.

The composition and humidity sensor, which is attached to the membrane, continuously measures the mass (x_i) and molar (y_i) fractions of all components, and the proportional controller applies water to the mixture as needed. Besides the mass flow (M_in), a transfer function (top right) determines the temperature of the applied water vapor from the current cell stack temperature.

Anode

Inside the anode (Figure 5), the hydrogen is split into protons and electrons, which chemically is an oxidation. The protons pass to the cathode through the membrane. The electrons flow through an external electrical circuit, generating the electrical current powering the attached load.

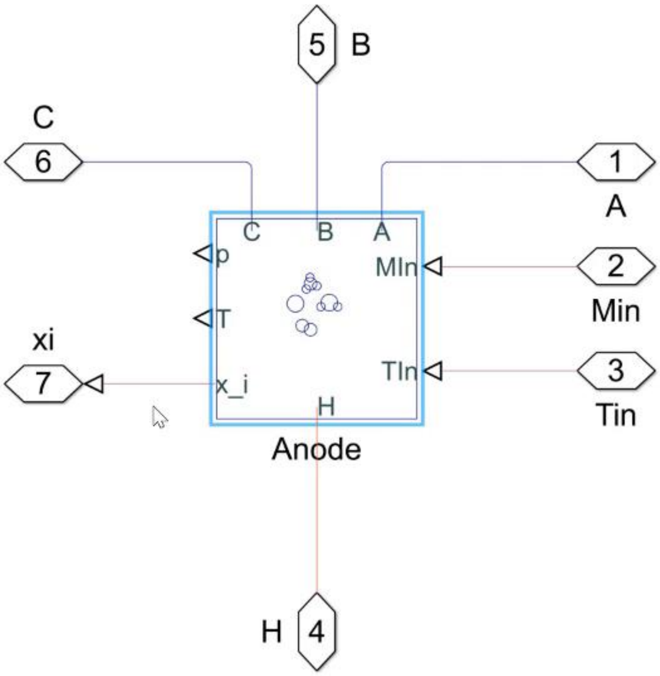
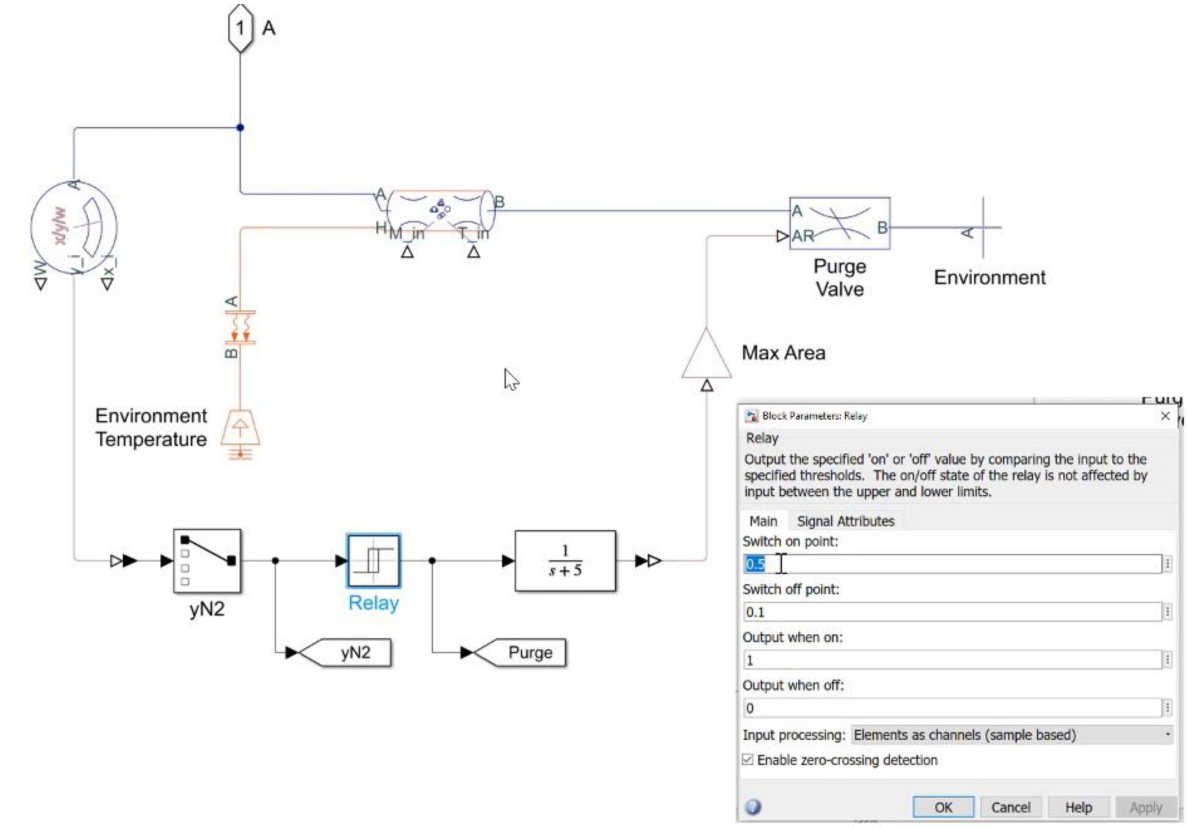


Figure 5. Anode gas channels subsystem.

The anode, also modeled as a constant volume chamber, has its input at port (C) and the gas leaves it at port (B). Port (A) is used for reading the temperature and pressure at the membrane, there is no flow over this element. Flow from the membrane is controlled using ports (Min) and (Tin). Port (H) exchanges heat with the cooling/heating system. Port (x_i) serves to get the mass fractions of individual gas components.

Exhaust and Purging System

During operation, nitrogen, in addition to protons and water, pass through the fuel cell membrane. Nitrogen accumulates at the anode, reducing the hydrogen fuel utilization, resulting in decreased power output. To mitigate this effect, the fuel cell system employs an exhaust at the anode to purge the system.



Block Parameters: Relay

Relay

Output the specified 'on' or 'off' value by comparing the input to the specified thresholds. The on/off state of the relay is not affected by input between the upper and lower limits.

Main | Signal Attributes

Switch on point: 0.5

Switch off point: 0.1

Output when on: 1

Output when off: 0

Input processing: Elements as channels (sample based)

☑ Enable zero-crossing detection

Figure 6. Anode exhaust with purging relay.

In this example, the reflow will be purged by a relay as soon as the nitrogen level reaches a molar fraction of 0.5 (Switch-on point in relay block parameters, Figure 6) and will stop at 0.1 (Switch-off point in relay block parameters). While purging is on, the purge valve will be completely open. While off, it will be fully closed.

Validating Controller Strategies: Purging Example

You can use Simscape to validate controller operation in this system. Simscape will record the outputs of all blocks during simulations. These can be inspected in the Simscape Results Explorer (Figure 7).

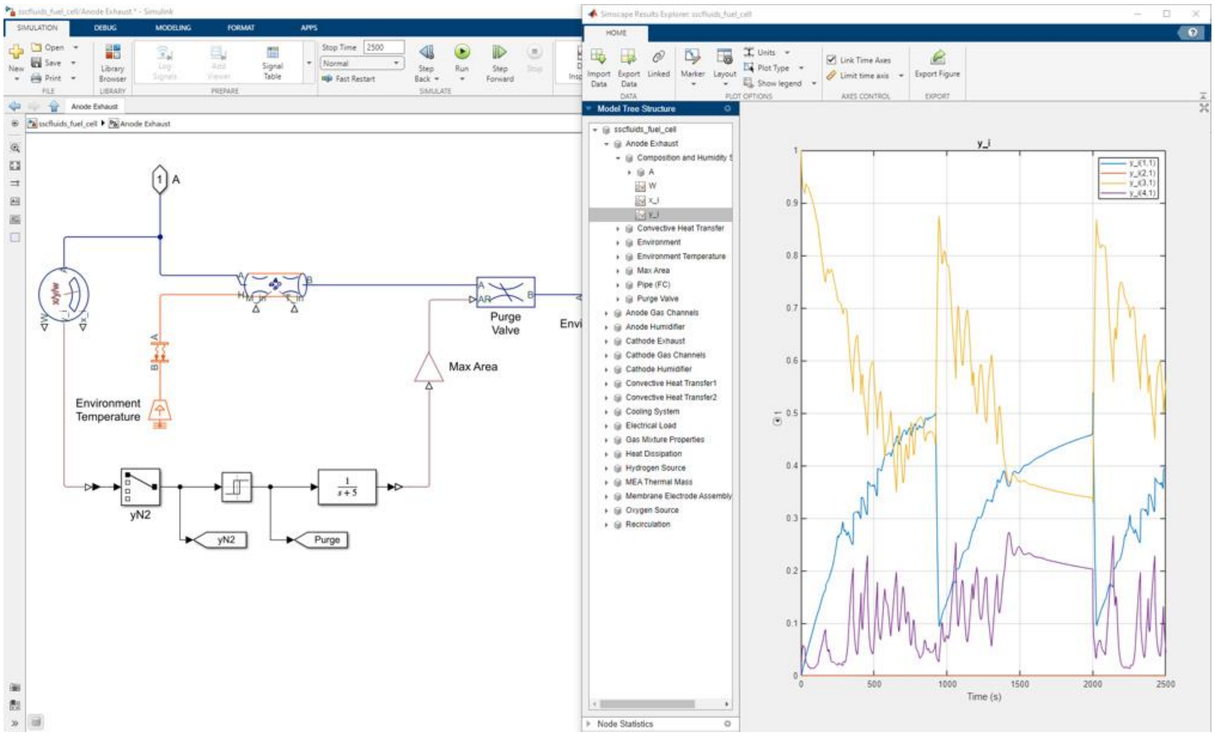


Figure 7. Purging element (left) with simulation results from the Simscape Results Explorer.

Here, we are looking at the molar fractions (y_i) of the gas species at port (A) of the composition and humidity sensor in the anode exhaust system during operation. The nitrogen level (blue line) is zero at the beginning. With rising nitrogen level, the hydrogen fraction (yellow line) decreases. When the nitrogen fraction reaches 0.5, the purging process starts and is stopped at 0.1 as desired.

At the same time, we observe that the water fraction (purple line) varies as controlled by the humidifier. And finally, the oxygen fraction (orange line) remains at zero, which is good as we never want oxygen and hydrogen together on the same side of the cell. The simulation results are a visual check on whether the purging strategy works, thereby validating the controller.

Air Intake

The cathode block (not shown) looks identical to the anode shown in Figure 5 and features the same ports and inputs. Inside it, oxygen as the reactant accepts the electrons flowing through the external electrical circuit and reacts with the protons from the membrane, forming water.

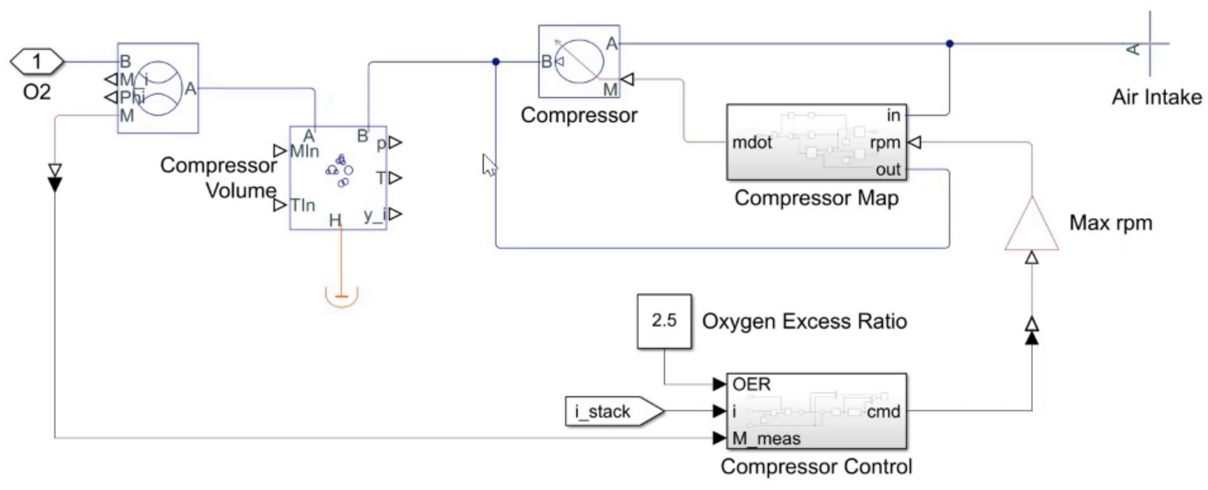


Figure 8. Air Intake Compressor with Controller.

The cathode side of the fuel cell system also differs from the anode side because it takes in air at ambient pressure and therefore needs a compressor to bring it to the required pressure inside the stack (Figure 8). The compressor has its own controller which acts on the current demanded by the electrical load (i_stack). No recirculation and purging systems are necessary as air is a readily available resource. Therefore, a simple exhaust is sufficient.

Cooling System

The cooling system is connected to the anode, cathode, and membrane (Figure 9). Liquid cooling is chosen due to its high efficiency. It consists of a tank, a pump, a heat exchanger, a radiator, and the pump controller which operates on the stack temperature, for which the setpoint is 80° C.

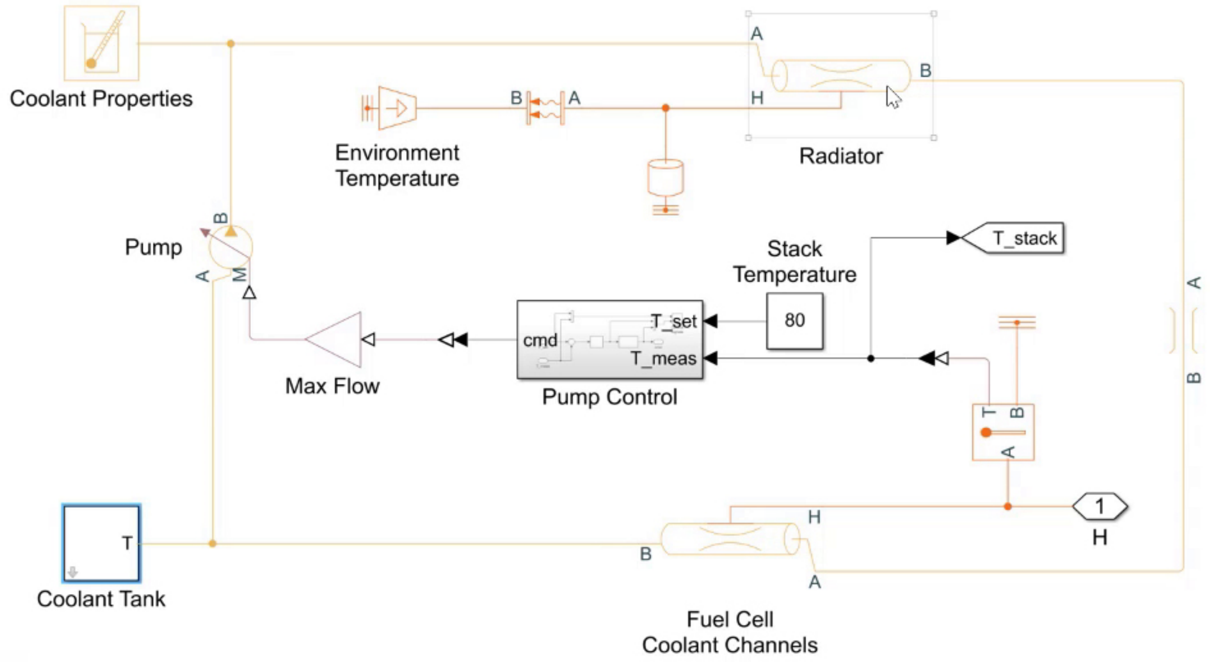
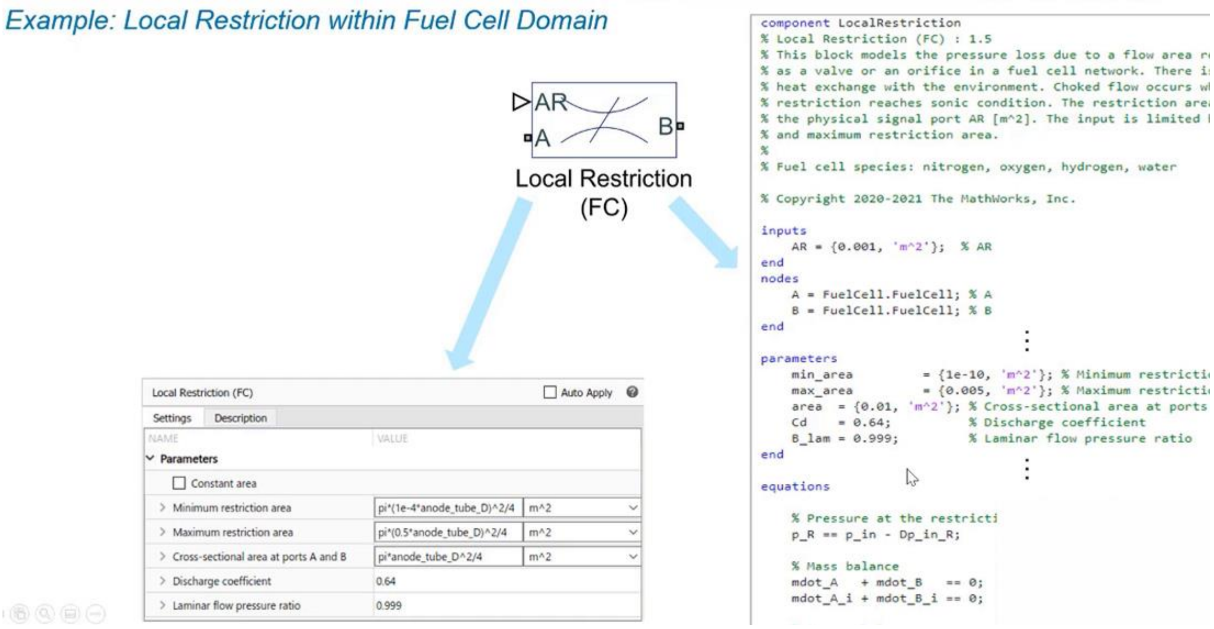


Figure 9. Liquid Cooling system.

Simscape Language: Modeling Custom Components and Domains

You can model your own custom components and domains using the Simscape language, which is based on MATLAB and supports the creation of Simscape blocks that can be used like any other library block (Figure 10). For simplicity, the example used here is the local restriction block from the custom fuel cell domain.



Example: Local Restriction within Fuel Cell Domain

Local Restriction (FC) ☐ Auto Apply

Settings | Description

NAME	VALUE	
Parameters		
☐ Constant area		
Minimum restriction area	pi*(1e-4*anode_tube_D)^2/4	m^2
Maximum restriction area	pi*(0.5*anode_tube_D)^2/4	m^2
Cross-sectional area at ports A and B	pi*anode_tube_D^2/4	m^2
Discharge coefficient	0.64	
Laminar flow pressure ratio	0.999	

```
component LocalRestriction
% Local Restriction (FC) : 1.5
% This block models the pressure loss due to a flow area r
% as a valve or an orifice in a fuel cell network. There i
% heat exchange with the environment. Choked flow occurs w
% restriction reaches sonic condition. The restriction are
% the physical signal port AR [m^2]. The input is limited 
% and maximum restriction area.
%
% Fuel cell species: nitrogen, oxygen, hydrogen, water

% Copyright 2020-2021 The MathWorks, Inc.

inputs
    AR = {0.001, 'm^2'};  % AR
end
nodes
    A = FuelCell.FuelCell; % A
    B = FuelCell.FuelCell; % B
end
                                  ⋮
parameters
    min_area          = {1e-10, 'm^2'}; % Minimum restricti
    max_area          = {0.005, 'm^2'}; % Maximum restricti
    area  = {0.01, 'm^2'}; % Cross-sectional area at ports
    Cd    = 0.64;          % Discharge coefficient
    B_lam = 0.999;         % Laminar flow pressure ratio
end
                                  ⋮
equations

    % Pressure at the restricti
    p_R == p_in - Dp_in_R;

    % Mass balance
    mdot_A   + mdot_B   == 0;
    mdot_A_i + mdot_B_i == 0;
```

Figure 10. Local restriction block component developed using Simscape language.

The source code (Figure 10, right) begins with either `component` or `domain`, followed by the name. It may contain a description of the block followed by the inputs it uses: AR, its nodes (A and B), and the parameters that can be configured using the parameter mask (bottom left).

Equations form the key part of a custom block. They express the behavior of the component, such as pressure at the restriction input and mass balance in this example. The blocks may also include energy balance or other equations.

If you work with partners or distribute your models and libraries, you may additionally protect your IP by saving them as binaries.

Simscape Blocks: Selecting Fidelity Levels for System Modeling

The model presented here uses a first principles approach with full gas dynamics. You can use this fidelity level for component sizing, control design and validation, for controller tuning, and for identifying concentrations of all gas species in the system's branches.

For some applications, a lower fidelity level is required or sufficient, either because individual simulations take too long or because only a rough behavior needs to be represented. For these cases, Simscape Electrical™ includes a simple fuel cell block reflecting voltage versus current behavior (Figure 11, bottom left).

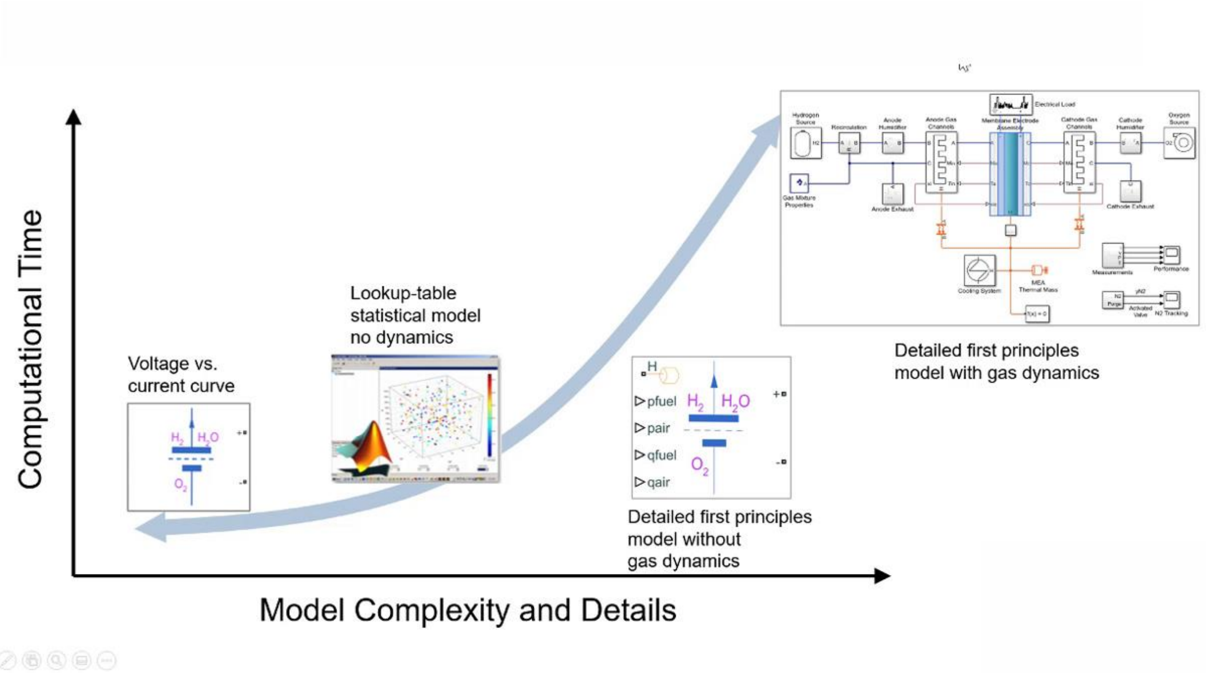


Figure 11. Computational time increases as a function of model complexity.

Simscape Electrical also contains more detailed models based on first principles but without gas dynamics (second from right) as well as lookup table–based statistical models (second from left) without dynamics. The latter do however require extensive measurements for gathering the required data.

Depending on the application, these different models enable you to select the model that best suits your needs in terms of level of detail and simulation speed. You can also extract a lookup-table–based model from the fully detailed model and use it to speed up simulations in later development stages without sacrificing accuracy. Together with other methods for simulation acceleration, such as parallelization or cloud computing, you can increase productivity and shorten development times.

Conclusion

Simscape offers options for modeling fuel cells at different fidelity levels. Individual components such as tanks, valves, the fuel stack, humidifiers, and compressors from different engineering domains can be accurately modeled together with their controllers.

Using custom domains and components, these models capture the behavior of complete fuel cell systems down to detailed thermodynamic and diffusion characteristics of mixed gases as well as in the thermo-liquid domain for temperature management and humidification.

You can use these simulation models for design, component parameter tuning, validation and code generation of controllers and logic, integration studies, and system and control parameter optimization.

Next Steps

Learn more about fuel cell models

Watch a webinar: Fuel Cell Integration for Electrified Propulsion