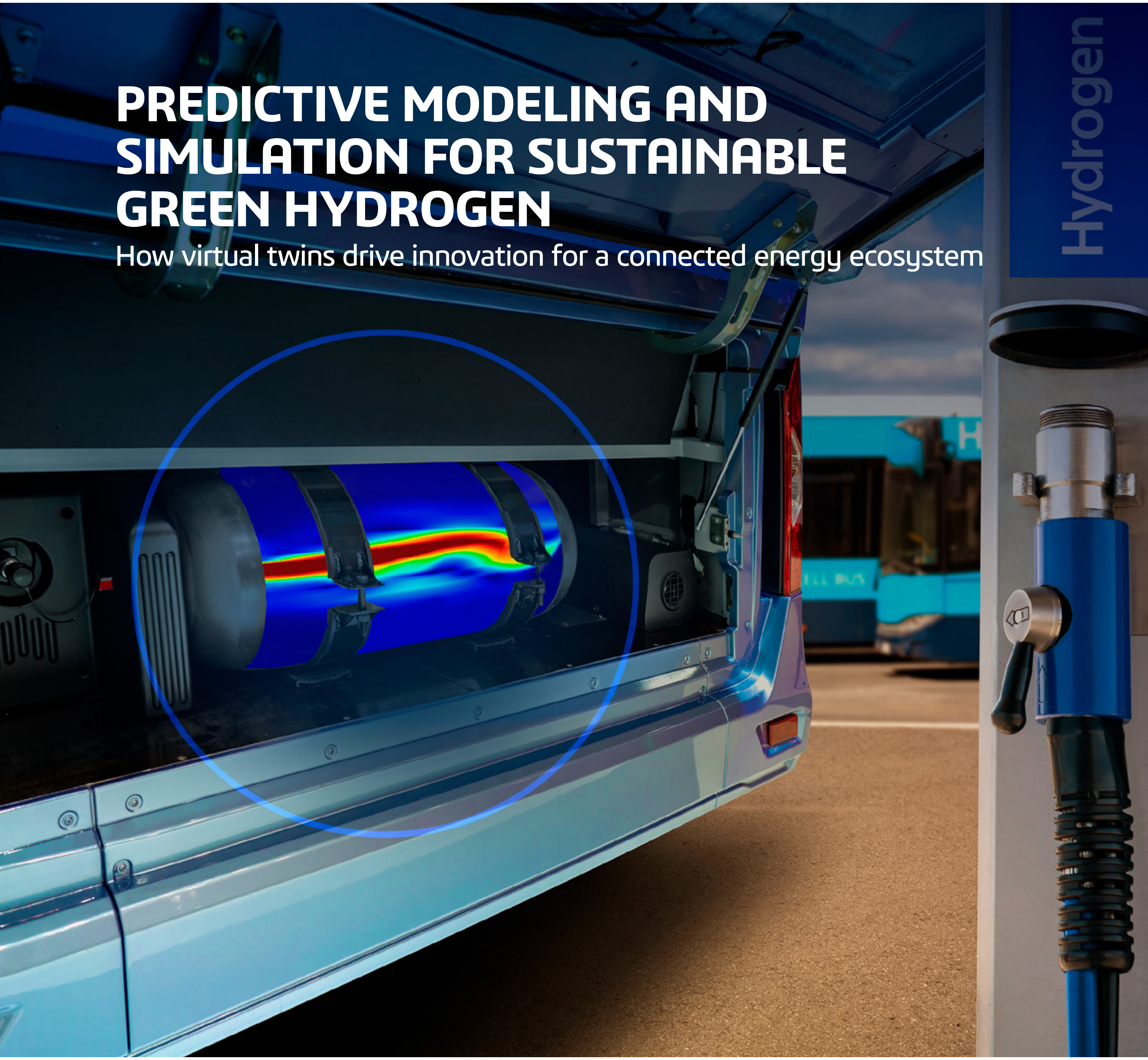
PREDICTIVE MODELING AND SIMULATION FOR SUSTAINABLE GREEN HYDROGEN

How virtual twins drive innovation for a connected energy ecosystem



HYDROGEN—A VIABLE ALTERNATIVE?

A fleet of hydrogen-powered Toyota Mirai vehicles took center stage as the official transport of the Paris 2024 Olympic Games. The company aims to sell 100,000 hydrogen vehicles per year by 2030[1].

Hydrogen promises to provide a clean, efficient system for storing and transporting energy. This lightweight, energy-dense element can carry big volumes of power indefinitely, with no carbon emissions when it's burned to release it, or converted to electricity in fuel cells. In conjunction with renewable energy, it has the potential to realize the vision of a truly zero-carbon economy.

Governments around the world are backing that vision with ambitious strategies and targets. For instance, the number of hydrogen-powered electric vehicles is set to increase from today's 16,000 to reach 13 million by 2030[2]. And total global hydrogen demand, currently around 90 million tons per year, will reach 585 million tons by 2050[3].

Delivering on hydrogen's promise will take innovation at every stage of the ecosystem:

Production

- Nature doesn't provide enough hydrogen, so we need to manufacture it—and the way we do that affects its environmental impact. Today, gray hydrogen, produced with high-carbon emissions, accounts for 95% of supply.
- A shift toward zero-carbon green hydrogen is essential to achieve clean energy targets. But this is currently the most expensive type of hydrogen to make. Production costs need to fall by around 75% to make it competitive with other forms of stored energy like coal or natural gas.

Storage and transport

- Hydrogen is a colorless, odorless and highly flammable gas that must be stored at high pressure and has an embrittling effect on metals.
- As well as negotiating complex vessel design, organizations must find ways to safely integrate hydrogen systems with existing pipeline infrastructure.

Usage

- Hydrogen users need tanks and filling stations that can safely handle the high pressures, temperature extremes and speeds needed for refueling.
- Efficient systems to convert hydrogen back into energy are also essential.

Different solutions must come together to make this ecosystem work as a whole. The problem is that it's difficult for an organization working on one aspect to coordinate its efforts with others—and that makes investment a risky prospect.

This whitepaper shows how predictive modeling and simulation, powered by the **3D**EXPERIENCE® platform, can power innovation as part of a connected whole.

1 https://www.greencarreports.com/news/1141566_toyota-more-hydrogen-than-solid-state-evs-by-2030

2 https://www.spglobal.com/commodity-insights/en/news-research/latest-news/electric-power/012420-fuel-cellevs-set-to-top-13-million-by-2030-as-hydrogen-scales-up-hydrogen-council

3 https://www.mckinsey.com/industries/oil-and-gas/our-insights/global-energy-perspective-2023-hydrogen-outlook

Different types of hydrogen and their environmental impacts

	 +Carbon Capture		
Grey hydrogen	Blue hydrogen	Yellow hydrogen	Green hydrogen
• Made by burning fossil fuels • Production emits large amounts of carbon	• Same production method as gray hydrogen • Carbon emissions are captured for reuse or storage	• Produced by water electrolysis • Uses electricity generated by nuclear power stations	• Produced by water electrolysis • Uses electricity from renewable sources
High carbon	**Low carbon**	**Zero carbon, but waste**	**Zero carbon, zero waste**

PREDICTIVE CAPABILITIES TO CONNECT THE ECOSYSTEM AND SHAPE THE FUTURE

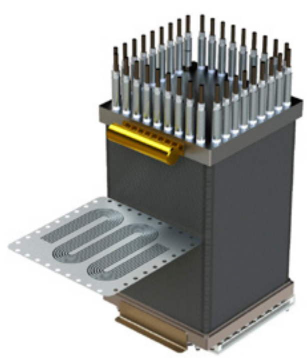
By integrating modeling and simulation—an approach known as MODSIM—on the **3D**EXPERIENCE platform, organizations can innovate efficiently and coordinate their efforts with others.

This approach allows them to create a virtual twin of the hydrogen ecosystem—a space where ideas can be tried out in the virtual world to see how they will work in the real one—and run predictive simulations, so that:

- Hydrogen handling equipment can be designed and engineered faster, with everyone collaborating on a single data model
- Multiscale simulations of materials, components and assemblies provide insights into hydrogen-material interactions, faster than laboratory testing
- Teams can use finite element analysis tools to assess complex, multiphysics, nonlinear behaviors and overcome technical barriers to blending hydrogen into existing infrastructure.

By testing their ideas in a virtual twin of the ecosystem, companies can innovate faster and reduce risk, with minimal need for costly and time-consuming physical prototypes.

PRODUCTION: ELECTROLYZER DESIGN AND SIMULATION



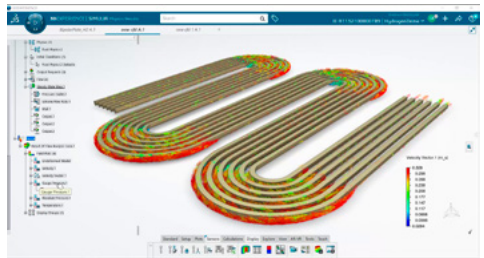
Water electrolysis—using electricity to split water into hydrogen and oxygen—is the cleanest way to produce hydrogen. Proton exchange membrane (PEM) water electrolyzers are especially suitable for solar or wind power because they can quickly adapt to varying generation levels. However, they can be 60% more expensive to produce than other types, and 40-50% of that cost comes from the electrolyzer stack:

- Each stack typically includes 100-200 PEM cells that up until now have required expensive catalysts like gold and platinum
- Each PEM cell is a complex sequence of layered bipolar plates, gaskets, anode and cathode collectors that is difficult to simulate
- Perfecting the design typically involves extensive, costly and time-consuming physical testing and every design change makes it necessary to re-manufacture the complete electrolyzer assembly.

MODSIM on the **3D**EXPERIENCE platform makes it possible to accelerate this design cycle and bring dramatic reductions in hydrogen production costs. This approach harmonizes all the data from different systems, providing a single model for everyone to work with and automated processes to help them work faster. It empowers engineers to carry out accurate and detailed multiphysics simulation earlier in the development cycle, so they can perfect their designs early on and dramatically reduce the need for physical tests.

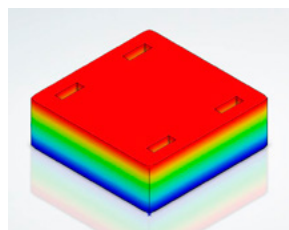
Example 1: Electrolyzer bipolar plate design

In this example, the user wants to refine the bipolar plate design for thermal and structural performance, as well as maximum production efficiency. This involves a delicate balance of physics, including making sure that the bolts are tight enough to avoid gas leakage and maximizing fluid flow rate, while keeping displacement, stress and plastic strain within allowable limits.



A complete geometric model of the electrolyzer stack has been created in the **3D**EXPERIENCE platform, including performance requirements for individual components. The user simply extracts the bipolar plate from this model and selects the geometry they want to work on.

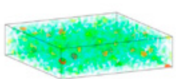
A finite element model of the plate is created, including material definitions and properties for the gaskets and diffusion layers. Any design changes are automatically reflected in the model and its mesh, without the need for pre-processing the model again. This ensures that essential components, like connections and fastenings, are retained.



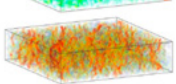
The platform provides unique RVE (representative volume element) based finite element analysis, which simplifies the simulation of bolt compression. This reduces the time and cost of optimizing the plate's geometric parameters and the number, spacing and load associated with bolts.

Next, a fluidic simulation is set up, targeting key performance indicators such as flow velocity, bubble formation, chemical reaction, temperature and pressure drop.

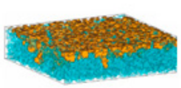
Pore sizes



Single-phase flow



Multi-phase flow

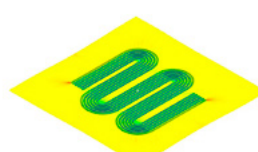


Users can also run microstructure analysis to gauge characteristics like permeability, diffusivity, electric and thermal conductivity. This enables them to choose the best materials for components like gas diffusion layers and bipolar plates, and design for optimal performance and efficiency.

The **3D**EXPERIENCE platform's automated processes allow hundreds of simulations to be run at the same time, providing immediate insights into issues such as predicted fatigue performance, maximum stress and strain, and expected lifetime and flow efficiency of the stack.

Example 2: Electrolyzer bipolar plate manufacturability

Obtaining a good virtual design is important, but ensuring it can actually be produced is equally crucial. MODSIM on the **3D**EXPERIENCE platform integrates parametric model design so design engineers can use simulation to make sure their designs meet manufacturing requirements. The manufacturing process can even be virtually represented to ensure performance objectives and manufacturability objectives are driven concurrently. This can drastically reduce the physical testing burden.



Users can incorporate computer-aided design (CAD) model parameters into simulations to create what-if studies for different manufacturing set-ups. This enables them to monitor manufacturing metrics for bi-polar plate stamping, such as thinning of sheet metal blanks and stress uniformity, and to evaluate alternative materials.

Crucially, all this data is reusable. As well as using the same CAD model to create design alternatives, development teams can reuse the manufacturing simulation to validate them. Immediate simulation results for every design change empowers them to achieve the optimal manufacturable design.

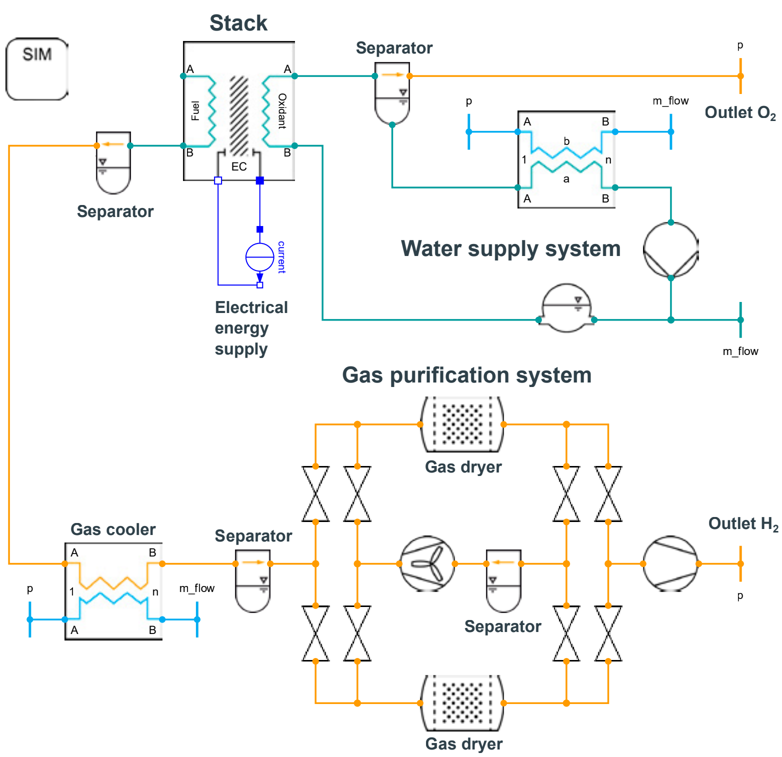
PRODUCTION: PLANT SYSTEM MODELING

Designing, integrating and operating all the systems and components for green hydrogen production is a complex, multidisciplinary process. There are many interdependencies to negotiate—for example, wind conditions for turbines must be synchronized with the supply of water and electricity so that electrolyzers can produce and store hydrogen in the most efficient way possible. System-wide monitoring and management is essential to ensure all components work together safely, efficiently and in compliance with regulatory requirements.

The **3D**EXPERIENCE platform provides a complete tool for modeling, simulating, testing and post-processing complex, integrated systems like these. Its Dymola (Dynamic Modeling Laboratory) makes it possible to create a virtual twin of the entire system, including supply sources like photovoltaic and wind farms, batteries, consumer electrical loads and distribution systems. Users can carry out multi-physics simulation at a system level and experiment with new configurations and operating conditions, to see how changes in one process will impact others.

Example: Simulation of hydrogen production system using Dymola Behavior Modeling

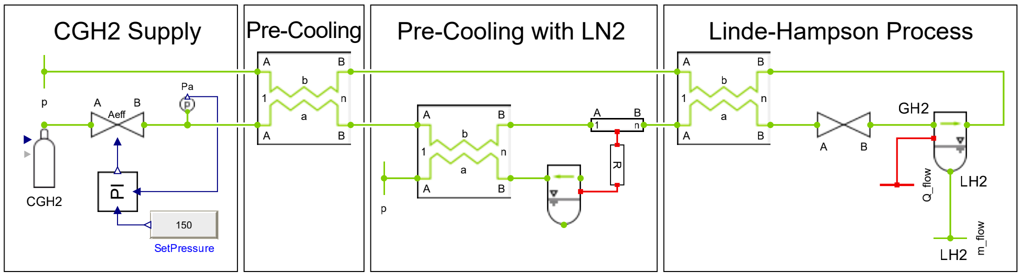
In this example, a company is planning to build a hydrogen production system. Before breaking ground, it creates a virtual twin of the entire project in the **3D**EXPERIENCE platform. This task is simplified by the Modelica Hydrogen library, which includes all the relevant components relating to hydrogen production and storage.



Modeling and simulation of PEM electrolysis systems. Image courtesy of TLK-Thermo GmbH.

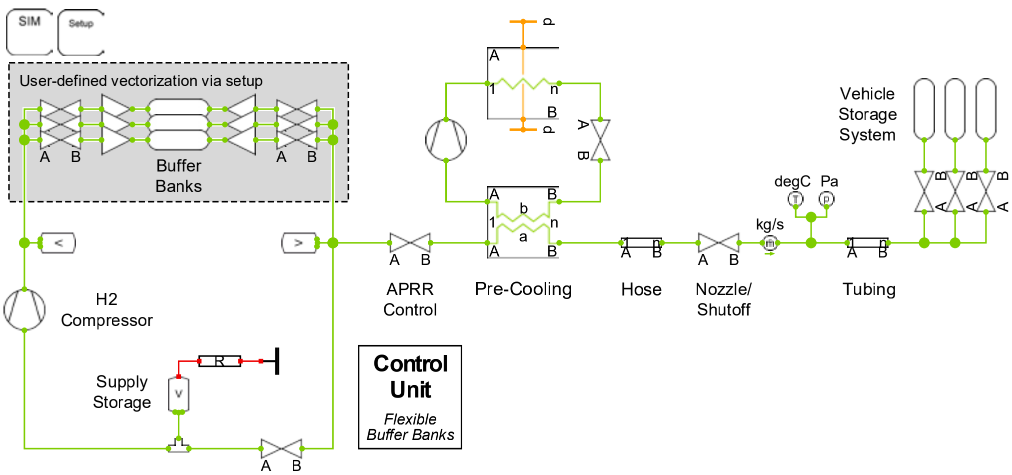
Modeling and simulating the hydrogen production system and processes allows the organization to operate the plant in a virtual environment and evaluate its performance in different conditions and compliance scenarios. This model provides:

- high-level energy analysis and integration across the system
- detailed insights for adapting the control strategy to deal with intermittent energy sources
- analysis and optimization of the entire system and its operating parameters, such as efficiency, water balance and thermal management.



Modeling and simulating the hydrogen liquefaction process. Image courtesy of TLK-Thermo GmbH.

Stakeholders across the system can use the same integrated data model to validate design choices, optimize system configurations and identify potential issues before building anything.



Modeling and simulation of hydrogen refueling stations. Image courtesy of TLK-Thermo GmbH.

Once the hydrogen production system is up and running, the company can use MODSIM to monitor performance in real time. Analyzing data from sensors and other sources allows the company to identify inefficiencies, predict maintenance needs and optimize production and distribution processes.

STORAGE AND TRANSPORT: TANK SEALING

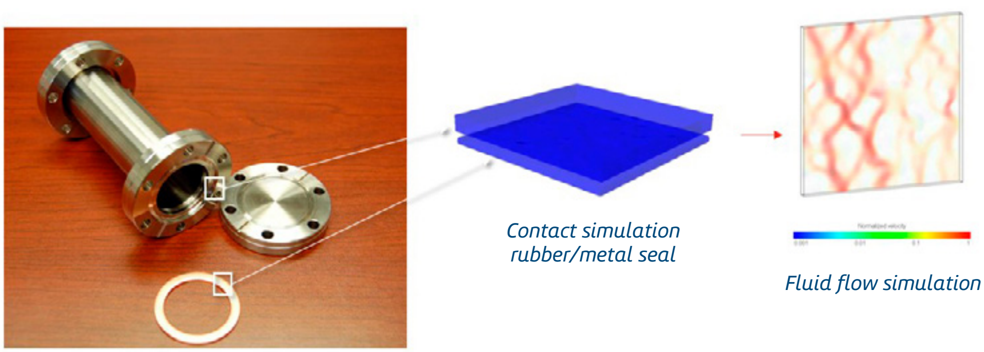
Existing infrastructure, such as natural gas pipelines, will play their part in storing and transporting green hydrogen. To do that safely, companies need to ensure that vessels, pipelines and pumping equipment can cope with the high pressures that hydrogen requires for storage. It takes detailed, multiphysics analysis of intricate pipeline systems to achieve that.

With Dassault Systèmes' multiscale simulation laboratory and Abaqus finite element analysis solution, organizations can accurately assess complex multiphysics and nonlinear characteristics of materials, components and assemblies. This allows them to:

- Overcome technical barriers to blending hydrogen into existing infrastructure
- Reduce the time it takes to design and engineer hydrogen handling equipment.

Example: Pipeline sealing

In this example, an engineer needs to make sure the equipment involved in filling the pipelines is securely sealed.



Contact simulation rubber/metal seal

Fluid flow simulation

Kkmurray, CC BY-SA 3.0 https://creativecommons.org/licenses/by-sa/3.0, via Wikipedia Commons

Abaqus is used to simulate the contact between the rubber and metal elements of the seal.

By connecting this simulation with one that shows fluid flow inside the system, the user can assess the seal's tightness and accurately predict any leaks or failures. This allows them to address potential issues before they become a problem.

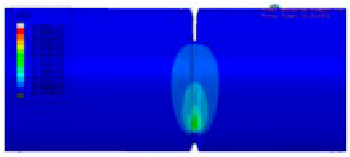
STORAGE AND TRANSPORT: EMBRITTLEMENT

Hydrogen atoms are small enough to permeate some metals, such as steel, iron and nickel. When the metal absorbs hydrogen, it becomes brittle and liable to cracking. To mitigate the risk of leakage, it's vital to understand how the complex interactions between hydrogen, materials, temperature and mechanical stresses will lead to embrittlement, and how cracks are likely to develop. Physical testing alone is too slow and expensive to achieve this level of insight efficiently.

MODSIM on the **3D**EXPERIENCE platform provides micro-level analysis of the interactions involved, with accurate predictions of where cracks will occur and how they will develop. This approach provides teams with a detailed understanding of hydrogen-material interactions, much faster than laboratory testing.

Example: Pipeline welding

Here, an engineer is assessing a pipeline weld using an end-to-end workflow solution for the design and analysis of hydrogen transportation pipelines. This workflow typically includes four steps.

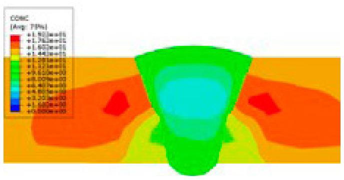


Welding Simulation

A thermal analysis is performed to determine the temperature-history of the weld. Then, based on the temperature and its rate of change, a metallurgical phase transformation model is used to predict microstructure formation. Temperature history can also be used to calculate thermal deformation and predict residual stress formation.

Molecular Simulation

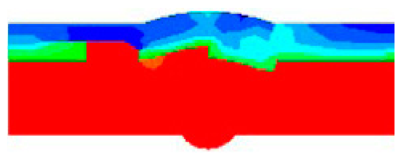
The user runs a molecular simulation using BIOVIA to show the diffusivity and solubility characteristics of material in and around the weld. This step uses alloy composition, pressure and the welding temperature history to identify the microstructures in which hydrogen will reside and their material properties. An Abaqus plug-in can be used to upscale these properties to the macroscopic level.



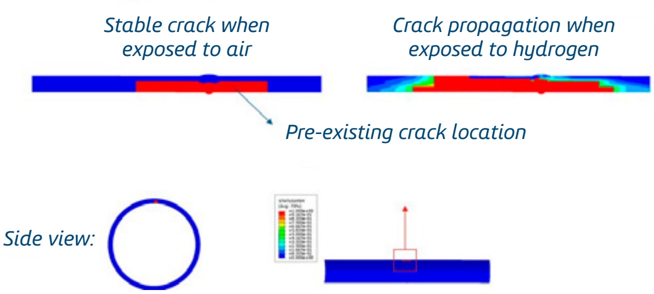
Hydrogen Diffusion

Next, hydrogen diffusion simulation shows the concentration of hydrogen in and near the weld. This is essential to evaluate hydrogen's impact on structural integrity, as it is a small element that can easily enter and migrate through materials, leading to material degradation. In metals especially, hydrogen can degrade the tensile strength, ductility and fracture resistance of materials.

Fracture modeling uses the hydrogen concentration levels from the diffusion simulation to predict how the presence of hydrogen will embrittle the pipeline and weld.



Hydrogen Embrittlement



In this example, the user has simulated the behavior of a pre-existing surface crack in the weld area, when exposed to air and hydrogen. The results show that the crack will remain stable when it is exposed to air, while hydrogen exposure will cause it to spread and penetrate the pipe.

By running accurate assessments like these to reveal how cracks will be affected by hydrogen concentration and operating pressure, the company can support decision-making to safely maximize the use of existing infrastructure.

USAGE: WOUND COMPOSITE TANK MODELING

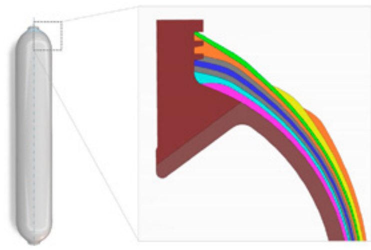
Hydrogen is a low-density gas, so it needs to be stored at very high pressure (350 to 700 bar) to achieve the required energy density for mobility applications. Composite overwrapped pressure vessels (COPVs), originally used for space exploration, are a popular means of achieving this. Structural integrity is crucial for these high-pressure storage tanks, and regulatory bodies worldwide have introduced stringent test protocols to prove they meet burst pressure requirements if they are dropped. Additionally, the polar bosses – the metal fittings at each end of the tank that connect it to the fuel cell and filling system—are critical safety elements.

Traditional development approaches, involving repeated physical testing, are too slow and costly. They also limit innovation because they don't provide enough insight on exactly how and why the tank's wound-composite layers fail. Simulation can help, but the varying material properties and complex winding of the filament bands, along with new polar boss designs that add geometric complexity, typically make this difficult to achieve.

A robust MODSIM-based methodology on the **3D**EXPERIENCE platform can overcome these challenges. It combines the capability to handle complex shapes and multiple composite lay-ups, with an intuitive interface for design engineers. This means users can quickly evaluate different design options for structural strength and durability in the virtual world, to ensure the best structural performance in the real one.

Example 1: Optimizing the design

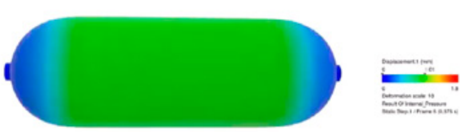
Let's say the design engineer wants to optimize a wound-filament tank design.



In CATIA, the user creates a 3D model of the tank's liners and polar bosses. Analytical equations based on design parameters such as wind-angle, lay-up thickness and turnaround radius are used to evaluate the thickness of each layer of the lay-up, and each layer is assigned fiber orientation and material behaviors. A mesh is automatically created, supporting a 3D finite element model that is easy to modify using design parameters.

Simulation is then set up to assess the tank's performance in areas such as boundary conditions and internal pressure.

Displacement



Stress distribution

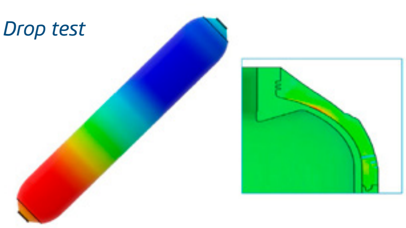
Here, a tank has been modeled to include the elastic, fail-stress and fail-strain properties of the laminations, as well as accurate metal properties according to the wind-angle of the composite at specific locations. Hashin Damage Criteria are defined for the composite layers, to give a clear picture of the material's behavior under stress and identify where and how any failure occurs.

The simulation reveals the displacement and stress distribution in the tank, along with potential failure points. Any changes made to improve the design are automatically meshed so the simulation can be run again, quickly and efficiently. This left-shifting of the product development cycle brings big productivity gains and makes it possible to develop novel tank designs faster.

Example 2: Certification impact testing

SIMULIA makes it possible to predict the tank's burst pressure with a static import analysis after the dynamic drop simulation. In addition, engineers can determine the composite winding angle, thickness and other layer parameters, and optimize the tank's weight, dimensions and thickness to maximize its resistance to impact.

Drop test



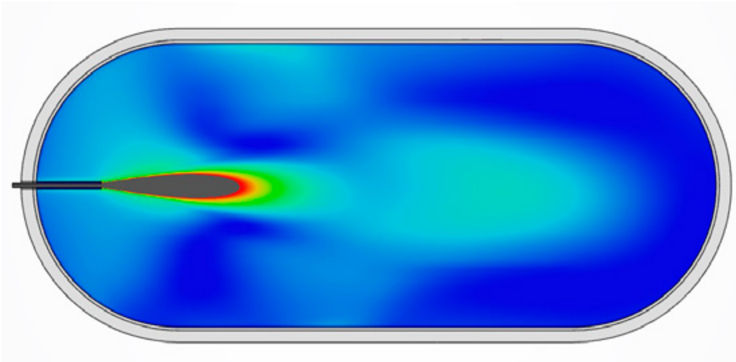
In this example, the simulation shows the tank being dropped onto a rigid floor surface at a 45-degree angle, at a velocity of five meters per second.

Each lamina of the tank was defined using elastic orthotropic material properties along with damage indicators based on the Hashin Damage Criteria. By reviewing these variables after the drop simulation, the user can accurately assess the impacted area of the tank, identify any problems and take steps to mitigate them.

USAGE: TANK FILLING

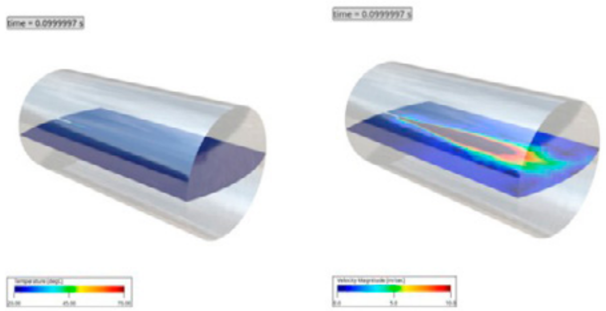
Safe operation, robust design and cost efficiency are the three golden rules when it comes to filling hydrogen tanks. Rapid tank-filling—ideally between 30 seconds and two minutes—is essential to maintain enough pressure and ensure that users can fill hydrogen-powered vehicles as easily as they can recharge or refill other types of vehicles. But rapid filling of hydrogen tanks brings steep increases in temperature, posing a challenge for the design of safe hydrogen-powered vehicles.

Careful choice of materials and components, such as inlet valves, is essential to ensure safe operation amid these extreme temperatures and optimize cost. A prototype-based design process is too slow and costly to achieve an optimized design.

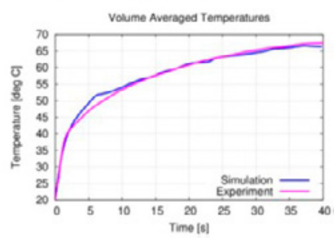


With MODSIM on the **3D**EXPERIENCE platform, engineers can simulate the filling of a hydrogen tank at high pressure. This makes it possible to identify the best materials, ply orientation and thickness to manage temperature and pressure, and to see how advanced valves can enhance the direction and fluctuation of the inlet flow.

Example: Tank filling fluid dynamics



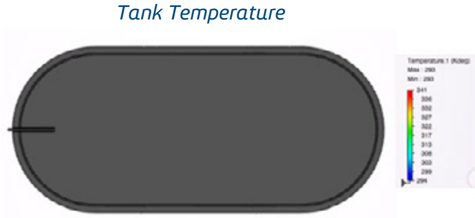
Probe averaged temperatures



In this example, the user has run transient computational fluid dynamics (CFD) simulations of tank filling temperature and velocity, using the **3D**EXPERIENCE's lattice Boltzmann approach. The temperature inside the tank is validated against an experiment, to ensure great accuracy in the model. Real gas modeling is used to accurately predict the pressure and temperature changes inside the tank.

External effects, like natural convection from weather conditions and the heating up of materials used for different layers, can also be included in the simulation. These transient simulations, with large eddy simulation modeling of turbulent effects, are particularly useful to help the engineer ensure accurate mixing within the tank.

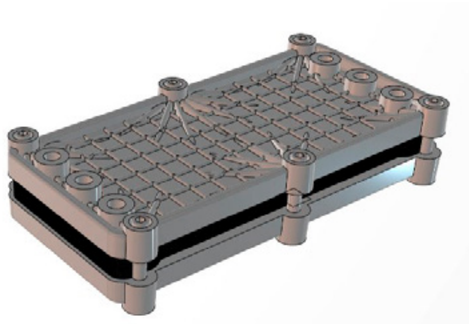
Tank Temperature



Tank Velocity

For even faster CFD analysis, the engineer can run simulations using a Reynolds Averaged Navier-Stokes FMK solver. This lower-cost simulation method also makes it possible to predict the exact temperature distribution in the tank. It provides a fast way to run many variations of inlet configurations or material selections.

USAGE: FUEL CELLS



Hydrogen-powered fuel cells are an effective alternative to Lithium-ion batteries in heavy-duty commercial vehicles, rail freight and marine applications—as long as they meet key usage criteria:

- Efficient energy conversion is essential to make hydrogen a cost-effective alternative to other fuel sources.
- To compete with internal combustion engines, hydrogen fuel cells must also be robust enough to support 150,000 miles of travel.

Typical PEM fuel cells (PEMFCs) are around 60% efficient, significantly higher than internal combustion engines. However, their performance can be adversely affected by the choice of materials in the gas diffusion layer, PEMs and catalysts, as well as their conditions. Evaluating newer materials and assemblies by testing is prohibitively expensive. Therefore, simulation methodologies that test these configurations are essential to ensure optimal efficiency and durability.

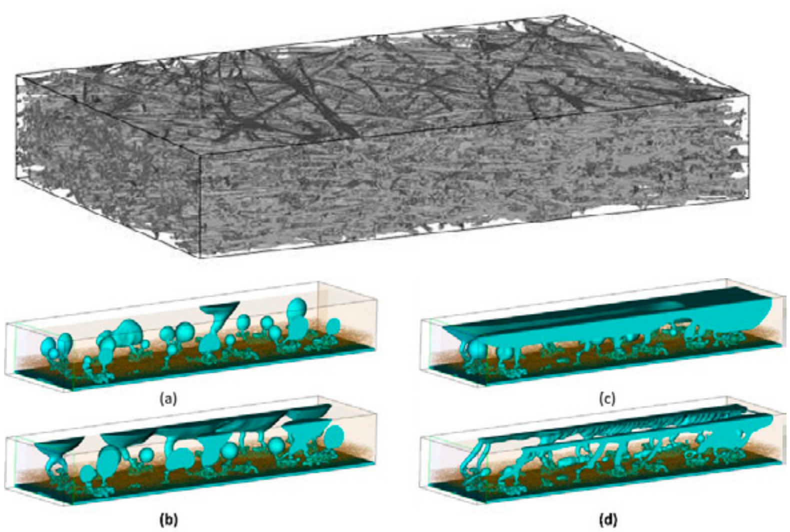
PEMFC workflows on the **3D**EXPERIENCE platform help users optimize the fuel cell's key physical aspects. On the cathode side of the cell, simulation of the two-phase flow through the gas diffusion layer and the bipolar plate is used to assess any water management issues. Meanwhile, fuel cell stack and finite element analysis determine the structure's strength and durability.

Example 1: Fuel cell water management

In this example, the design engineer is using computational fluid dynamics to simulate the flow of air and water through the cell's entire cathode-side bipolar plate and gas diffusion layer. X-ray micro-tomography scanning has been used to provide the cell's exact geometry. In addition, Lattice Boltzmann two-phase flow and upscaling—two technologies unique to the **3D**EXPERIENCE platform—are used to map the results from a patch to the whole of the bipolar plate.

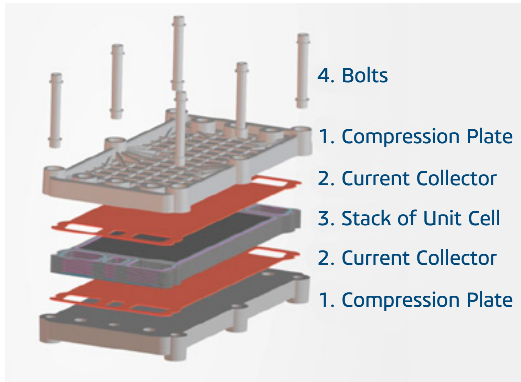
Simulated flow patterns identify water breakout points, water distribution and channel pressure drop. These outputs are used to evaluate whether the design:

- enables adequate hydration of the gas diffusion layer
- has the correct two-phase flow regime to deliver the mass flow rates and pressure drops needed for optimal operation and efficiency.



Simulation of the gas diffusion layer geometry (above), with the two-phase flow through the bipolar plate (below)

Example 2: Fuel cell structural finite element analysis



To determine the strength and durability of the fuel cell stack, the user runs a structural simulation to calculate stresses, displacements and durability for the entire structure.

This is made possible by combining the Abaqus finite element analysis solver with Representative Volume Element—a tool that enables a reduction in model size so the whole fuel cell assembly can be simulated.

Using this workflow, the design engineer can evaluate whether the material selection and assembly of the fuel cell meet requirements for permissible stresses on components, overall durability and warranties. This enables them to develop longer-lasting fuel cells, which will decrease the cost of ownership.

FUELING A CLEAN ENERGY FUTURE

Creating a whole ecosystem is a daunting task if you go it alone. It becomes much more achievable —and affordable—when different parties can connect so that each plays their part in creating a greater whole.

Innovate faster

The **3D**EXPERIENCE platform provides a complete, cloud-based suite of applications that enable fast, high-quality and sustainable product development, protected by state-of-the-art cloud security and privacy controls.

Connect the system

Managing everything in the **3D**EXPERIENCE platform brings enhanced connectivity between component design and system performance, enabling greater efficiency and lower cost of ownership.

Collaborate better

Designed for collaboration, the **3D**EXPERIENCE platform connects internal and external stakeholders across the ecosystem, to help them progress together in a synchronized way.

Design safer

MODSIM brings the capability to predict complex behaviors and interactions at all levels, from materials to plant infrastructure, so organizations can design solutions for maximum safety and efficiency.

Drive affordability

Predictive simulation dramatically reduces the need for physical prototypes and testing, making it more affordable to realize hydrogen's promise of clean energy storage.

Crucially, nobody needs to innovate alone. With secure collaboration and powerful cloud computing, ideas and knowledge can be shared and reused so organizations can make sure their innovations will work together. This optimized connectivity empowers companies to speed up progress toward our clean energy future.

To learn more about how the **3D**EXPERIENCE platform can help you connect to the hydrogen ecosystem, contact us.

Dassault Systèmes is a catalyst for human progress. Since 1981, the company has pioneered virtual worlds to improve real life for consumers, patients and citizens.

With Dassault Systèmes' **3D**EXPERIENCE platform, 370 000 customers of all sizes, in all industries, can collaborate, imagine and create sustainable innovations that drive meaningful impact.

For more information, visit: **www.3ds.com**

Virtual Worlds for Real Life

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