

EXPLORING HYDROGEN TANK FILLING DYNAMICS

Convergent Science White Paper

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INTRODUCTION AND MOTIVATION

With the push toward net-zero emissions, renewable technologies are poised to play a significant role in the future of the transportation and energy sectors. While multiple technologies have the potential to help move us toward our goal, few show as much promise as hydrogen. Hydrogen can help address issues related to energy security, pollution, emissions reduction, and sustainability across many industrial sectors, making it a key focus of research and development efforts. Additionally, there is a growing interest in green hydrogen production and storage technologies, which could position hydrogen as one of the primary fuel sources for both industrial processes and transportation.

Hydrogen offers a number of advantages over conventional fuels, including:

1. Reduced carbon emissions: Technologies powered by hydrogen, a carbon-free energy carrier, can produce significantly less use-phase carbon emissions compared to traditional fossil fuels.
2. Abundance and renewability: Hydrogen is the most abundant element in the universe and can be produced from a variety of sources, including water, biomass, and natural gas.
3. Versatility: Hydrogen can be stored as a gas or liquid, making it a candidate for a wide variety of applications, including transportation, power generation, and industrial processes.

Storage and transportation are core components of the hydrogen supply chain. With hydrogen production being scaled up for industrial and transportation needs, safe and reliable storage methods are becoming increasingly important. Engineers must account for the highly diffusive and corrosive nature of hydrogen, which makes it prone to leaking. Furthermore, the thermodynamic properties of hydrogen, such as the negative Joule-Thompson effect, differ substantially from other fuels, requiring engineers to rethink traditional storage infrastructure.

Designing tanks to store hydrogen under cryogenic and normal conditions presents some significant challenges:

1. Extreme sensitivity to the environment leads to large fluctuations in the thermophysical properties of hydrogen.
2. The low compressibility of hydrogen means tanks need to withstand high pressures during the filling process.
3. The stability of the thermal environment is affected by the presence of heat pockets, which impact the thermal stress distribution within the tank. Localized thermal stresses can be a safety hazard because they can compromise the integrity of the tank structure.

To tackle these issues, we must assess the design of the tank from multiple perspectives: thermal stability, ability to diffuse and degenerate the thermal pockets, and mechanical strength, which must be capable of withstanding local thermal gradients and stress due to high storage pressures.

Computational fluid dynamics (CFD) is a powerful tool that can help address some of the primary challenges associated with using hydrogen as a fuel. CFD can provide valuable insight into the behavior of fluids and gases in different environments, including the transport and combustion of hydrogen. CFD simulations can be used to optimize the design of hydrogen fuel systems, such as fuel cells, storage tanks, and delivery systems. By simulating the flow of hydrogen and air in different configurations and conditions, we can identify areas for improvement in the fuel system design to increase efficiency and reduce emissions. We can also use CFD to simulate the behavior of hydrogen in different storage and transportation systems, such as pipelines or tanks. This can help us identify potential safety hazards and optimize the design of the storage and transportation systems to minimize the risk of accidents.

In this white paper, we focus on modeling gaseous hydrogen storage using CONVERGE CFD software. We'll highlight the benefits of CFD in understanding the tank filling (and emptying) physics and discuss how these studies are important in the design of safe storage systems. We start with an overview of the case study and the numerical setup, highlighting the most relevant settings and features. We then present the results of the study and conclude with some final remarks and outlook.

SIMULATING HYDROGEN STORAGE IN CONVERGE

CONVERGE offers a suite of robust, versatile features relevant to hydrogen tank filling simulations:

1. Autonomous meshing removes the mesh generation bottleneck and creates a high-quality cut-cell mesh for any complex geometry at runtime. Adaptive Mesh Refinement (AMR) adjusts the mesh resolution throughout the simulation to capture the flow patterns and reduce numerical diffusion.
2. The thermodynamic properties of hydrogen can be modeled via real gas equations or using thermodynamic tables generated with the click of a button.
3. A wide selection of turbulence models can be used to capture the flow interaction within the storage unit, from jet expansion at the injector to circulation within the broader system.
4. Conjugate heat transfer (CHT) can solve the heat exchange between the various fluid and solid components in the system.

5. Key quantities can be extracted for post-processing, including both local values and averages over a portion or the entirety of the computational domain.
6. CONVERGE couples with external software (e.g., Abaqus) to accurately capture the thermal stresses and corresponding deformations.

HYTRANSFER PROJECT VALIDATION CASE

With the growing interest in hydrogen fuel systems, multiple research initiatives supported by government funding are investigating and validating the proof-of-concepts for different stages of the hydrogen ecosystem. One such project is HyTransfer,[1] which was funded by the European Union to study the key physics in the hydrogen filling process and provide guidelines on how to achieve an efficient filling strategy and tank design for commercial vehicles. Several experiments were conducted to this end, and the critical parameters were identified and documented.

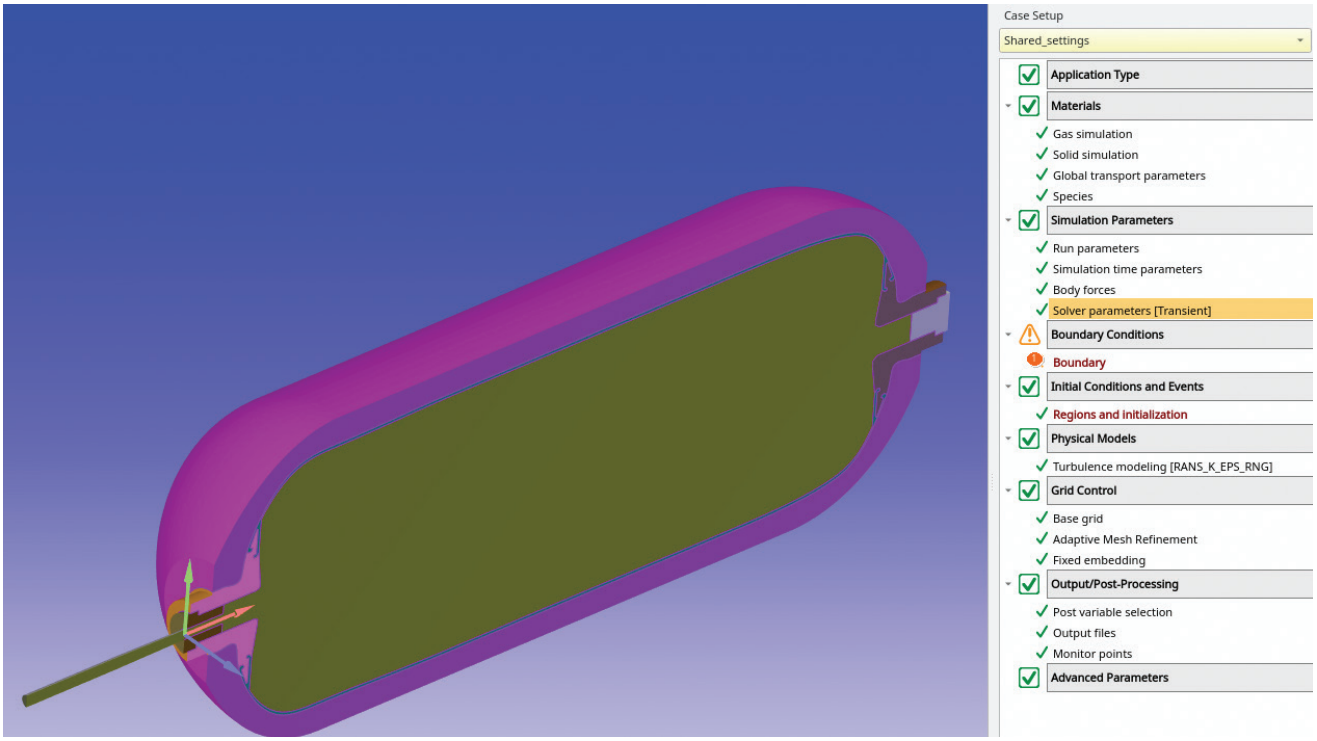
To demonstrate the value of CONVERGE for hydrogen storage problems, we conducted a validation study based on the experimental data available for public access in the framework of the HyTransfer project.

The Hexagon 36 *L* Type IV tank, considered in this study, consists of a polymer liner encased in a composite wrapping to provide the necessary structural strength to withstand the large pressures. The tank has been designed to withstand a nominal pressure of 70 *MPa*. The liner has a thickness of approximately 4 *mm*. Data for two different injector diameters, 3 *mm* and 10 *mm*, were available; the 10 *mm* injector diameter is considered here. To reduce the overall computational costs, we simulated only half of the horizontal tank domain, as proposed in the literature.[2,3,4] We provided the inlet mass flow rate profile and monitored the development of the tank pressure from the initial state. Several measurement points were placed within the tank to assess the fluid and solid temperatures at different locations.[1]

CONVERGE SIMULATION SETUP

In CONVERGE Studio, the user-friendly graphical user interface for CONVERGE, you can prepare your geometry, define regions, and set up your case (Figure 1). You can import a native CAD format or STL file of your geometry into CONVERGE Studio and take advantage of a vast array of geometry manipulation and repair tools. With the CoolProp utility integrated in CONVERGE Studio, you can generate the fluid properties of hydrogen over the required temperature and pressure range at user-defined intervals.

Additionally, CONVERGE provides the option to use real gas properties with the appropriate corrections for compressible fluids. This is a key feature for simulations involving hydrogen, as its behavior tends to deviate significantly from ideal gas representations.



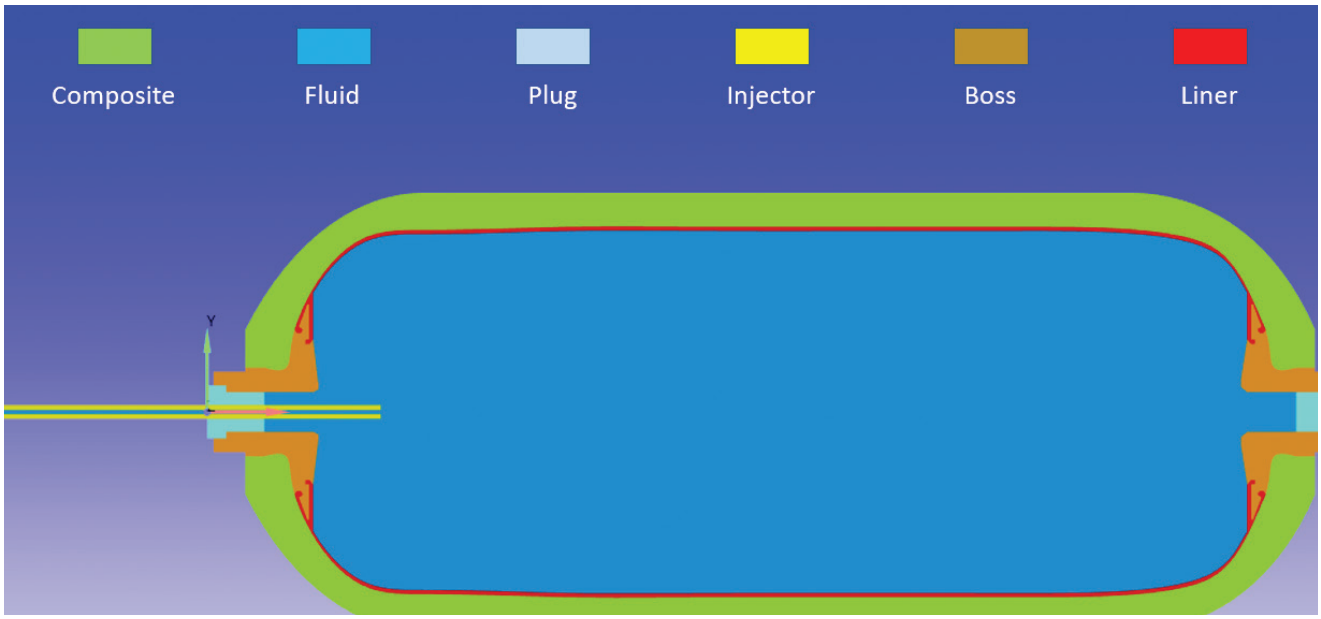


Figure 1: *Top: CONVERGE Studio screenshot showing the tank geometry and the case setup tree; only the activated physical models are shown. Bottom: The different regions defined in the model for material and physical properties.*

We use the density-based PISO solver with proper tolerances to achieve rapid convergence at each time-step (details in Table I). The heat exchange between the fluid and solid domains is modeled with CONVERGE's CHT approach. With proper thermodynamic and material properties, the heat fluxes between the different regions are captured accurately.

Solver	PISO density-based Compressible
Turbulence model	RNG k-epsilon
Wall treatment	Automatic wall function
Fluid properties	Tabulated fluid properties (CoolProp)
Spatial and temporal discretization	Finite-volume second-order central in space First-order in time

Table 1: *CONVERGE solver settings and models.*

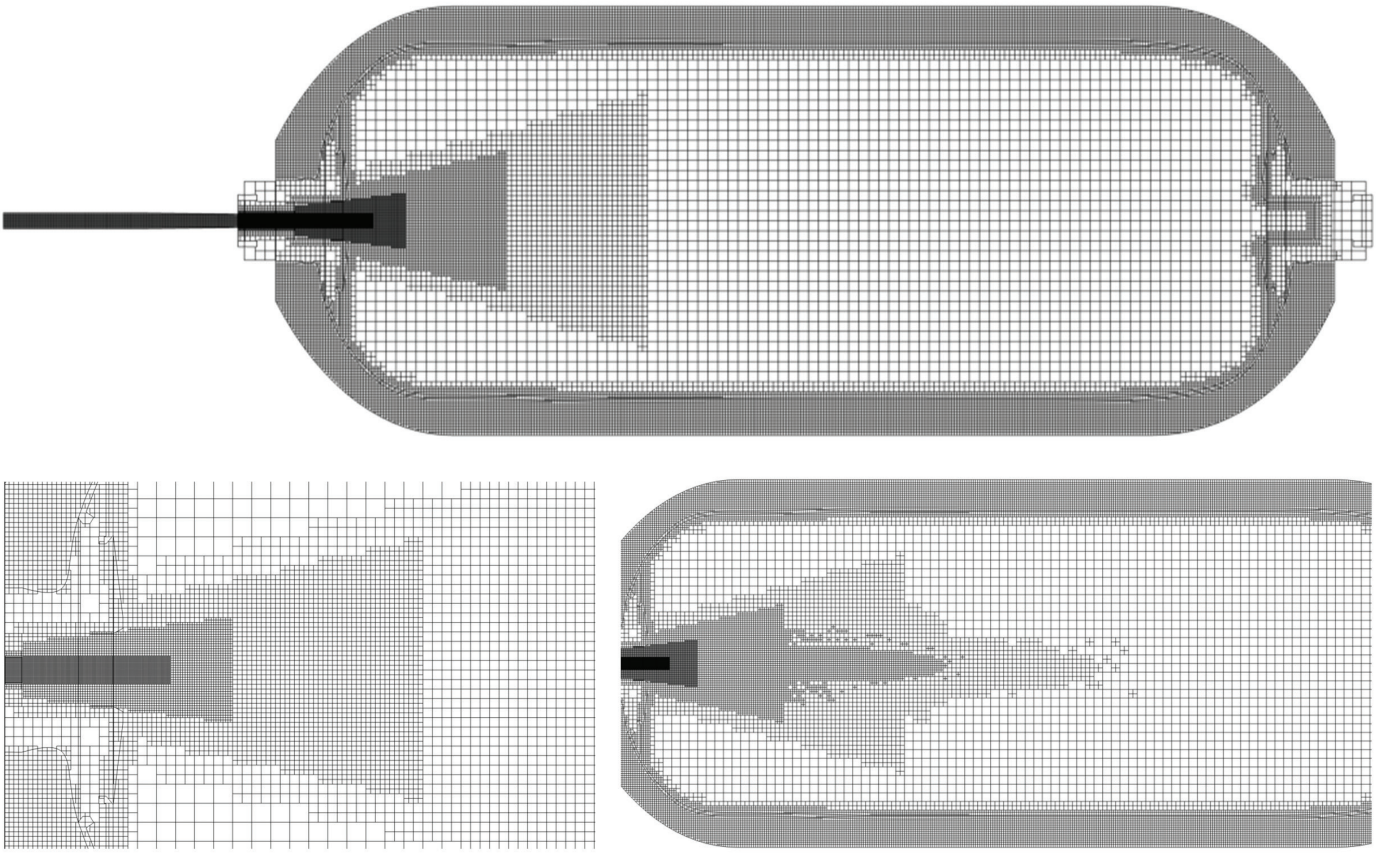


Figure 2: *Mesh distribution used for this study. Top: Cut-cell mesh with fixed mesh embedding. Lower left: Mesh embedding at the injector region. Lower right: Velocity-based AMR to capture the jet spreading.*

Region	Cell sizes [min. – max.] (*mm*)
Fluid	0.9375-15
Composite	3.75
Liner	1.875-3.75
Boss	3.75-7.5
Plug	3.75-7.5
Injector	0.46875-0.9375

Table 2: *Mesh size distribution in different regions. The minimum and maximum cell sizes are provided where applicable.*

As the injector diameter used for hydrogen tanks typically ranges from 3*mm*–10*mm*, the incoming flow velocity can easily reach up to 300 *m/s*. Higher jet penetration plays a crucial role in the circulation within the tank (shown in Figure 2); mesh embedding used in conjunction with AMR can capture the jet profile with good accuracy. The mesh size distributions used in the different simulation regions are provided in Table 2, and the total cell count is given in Figure 3.

To get the appropriate jet penetration and reduce the spreading over-prediction, the RNG k-epsilon constant $C_{\varepsilon 1}$ in the turbulence model is modified as suggested by other researchers.[2,3,4] Monitor points are inserted at the locations specified in the experimental setup, and the quantities are plotted using the in-built post-processing utility in CONVERGE Studio.

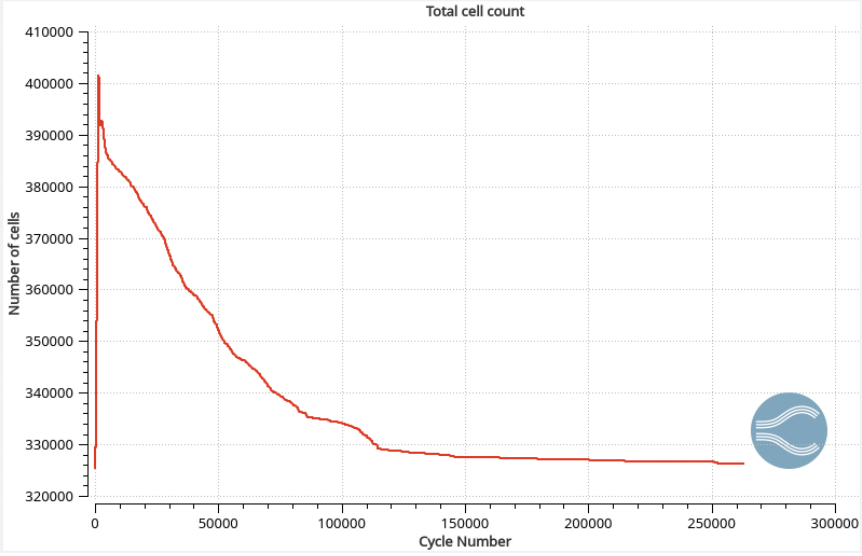


Figure 3: *Number of finite volume cells throughout the simulation runtime.*

RESULTS AND DISCUSSION

In this section, we analyze the numerical results obtained from our hydrogen tank filling study with the 10 *mm* injector diameter configuration.

The velocity contours in Figure 4 show the high penetration of the hydrogen jet during the filling process. It is important to select an appropriate turbulence model to capture the jet penetration and spreading. The initially high velocity jet subsides as the filling progresses due to the compression of hydrogen.

The flapping motion of the jet can indicate significant flow circulation within the tank, which plays an important role in the redistribution of the thermal gradients. Hot pockets are observed toward the injection side of the tank because of the circulation within the tank (Figure 5).

CONVERGE includes the capability to monitor desired fields in regions of interest in the domain, and the data can be analyzed through built-in post-processing tools. The simulations accurately capture the pressure increase within the tank compared to the experimental data,[1] as shown in Figure 6.

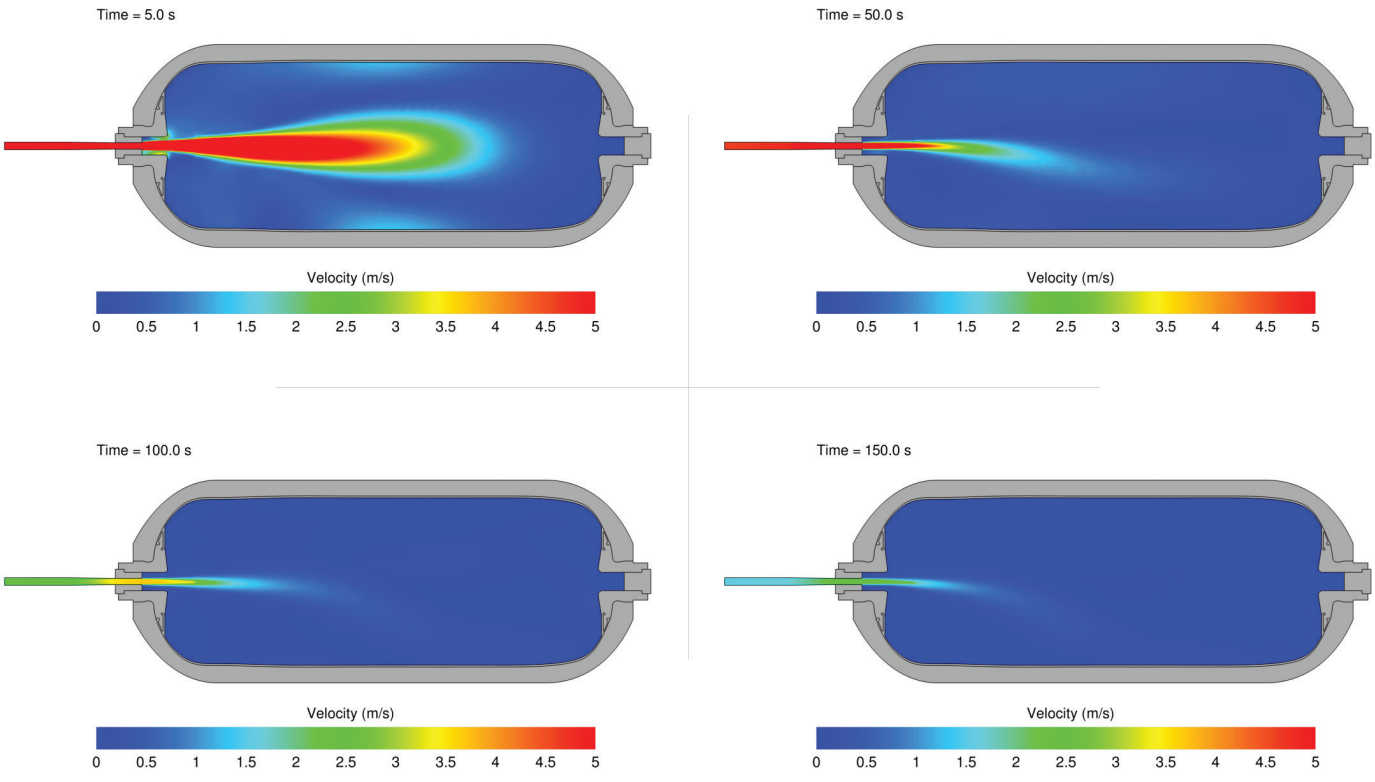


Figure 4: *Velocity contours of the hydrogen filling process with a 10mm injector diameter at 5, 10, 100, and 150 seconds.*

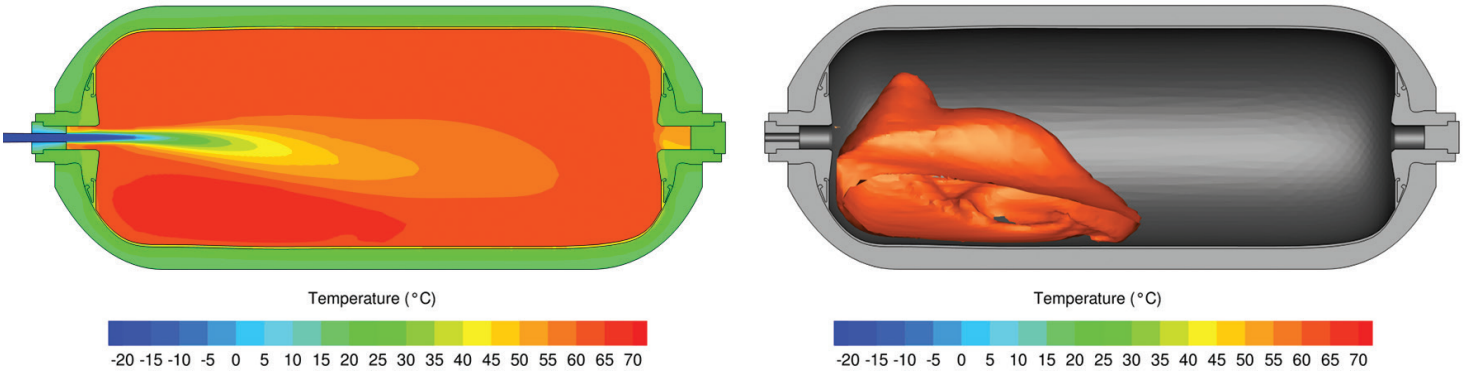


Figure 5: *Left: Temperature contour within the tank showing the different temperature regions. Right: The iso-contour of T = 65°C showing the location of the hot pocket.*

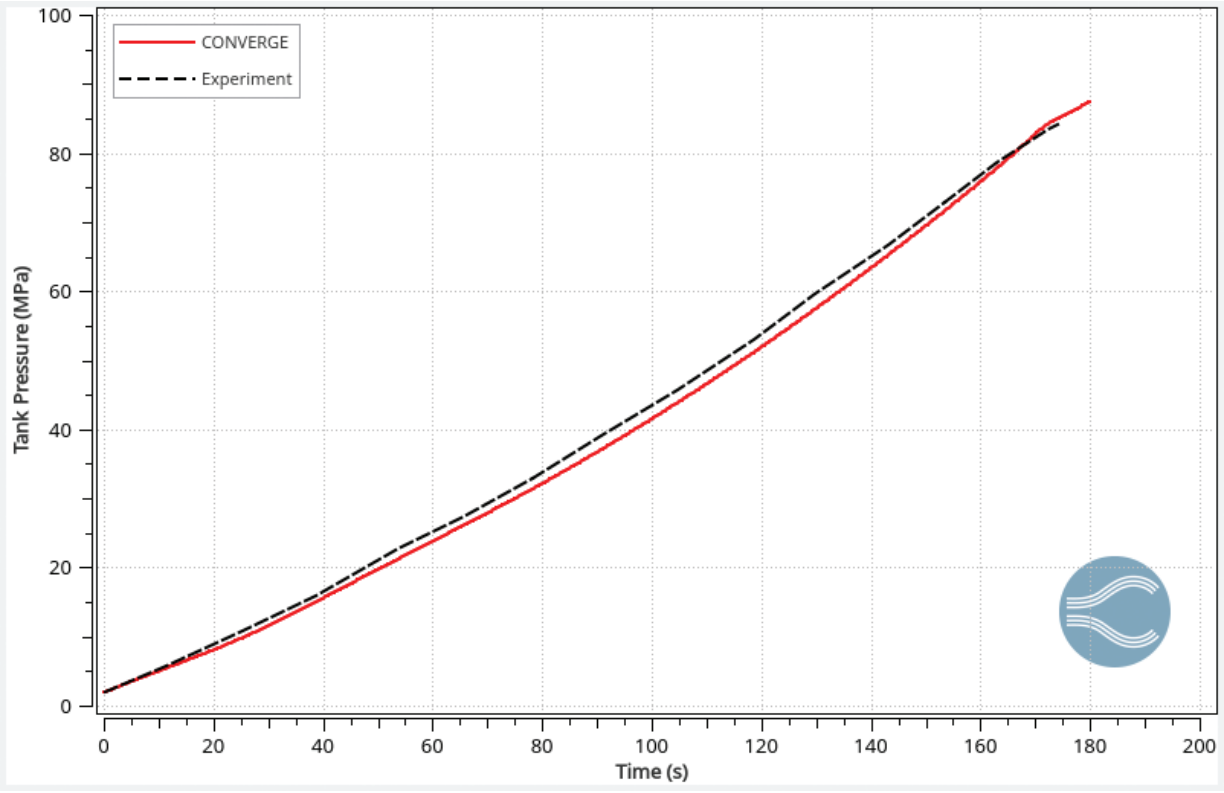


Figure 6: *The tank pressure measured at the rear-end of the tank. The experimental data is taken from [1].*

The temperature profiles within the tank also agree well with the experimental data (Figure 7), demonstrating that CONVERGE can capture the complex thermodynamics of hydrogen. Thermocouple TT1 is located in the lower section of the tank, while thermocouple TT5 is located in the upper section. The reading at TT5 is higher than TT1 because of the thermal stratification that is prone to occur as a result of long filling times. As the filling progresses, the jet velocity decreases and the circulation within the tank stabilizes, leading to thermal stratification as observed by the two thermocouple readings.

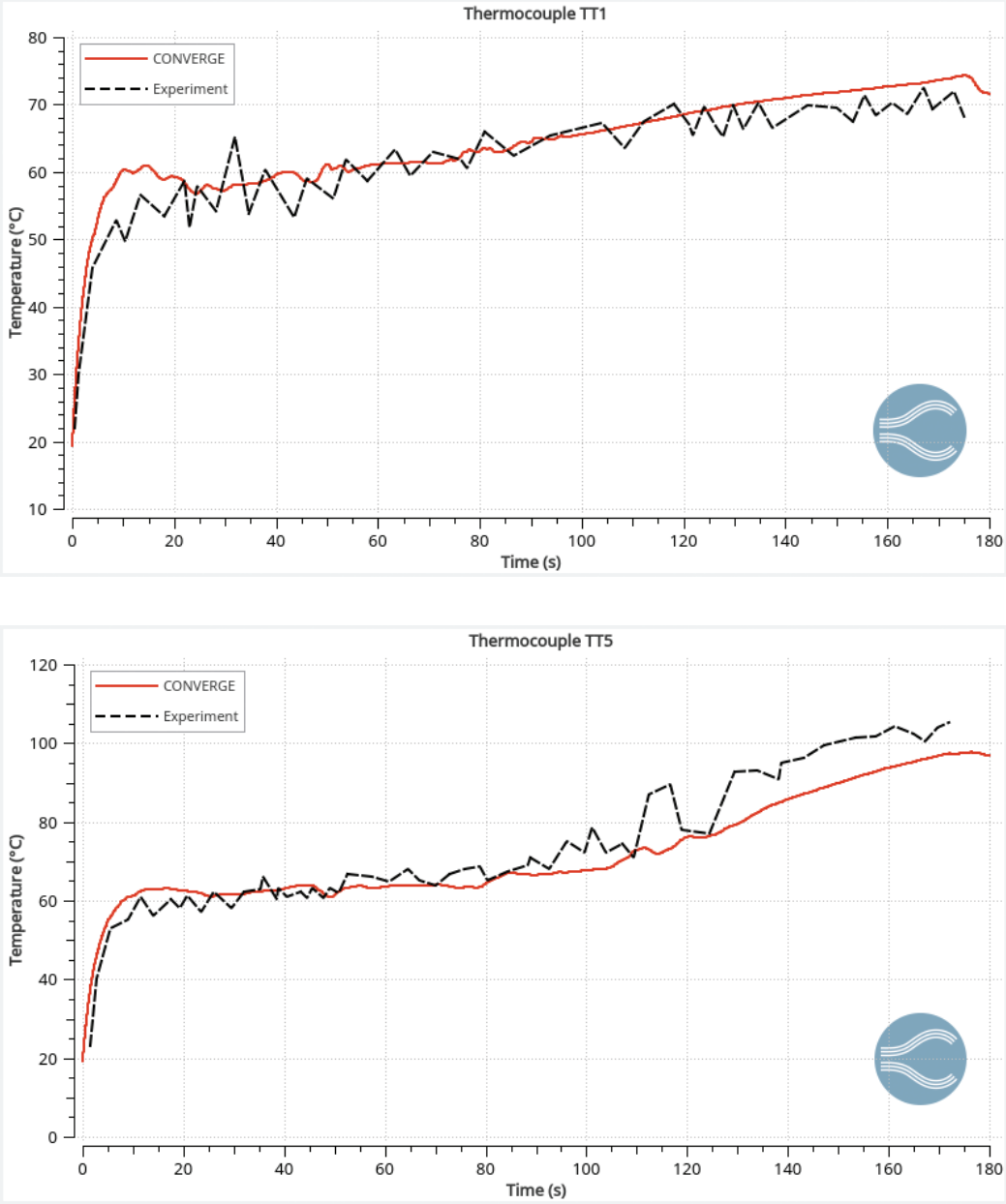


Figure 7: *Thermocouple readings at locations TT1 (top) and TT5 (bottom). Temperature trends agree well with experimental data [1].*

Another important design factor is the tank material. Ideally, we want a lightweight system with excellent thermal integrity and strength. To achieve these characteristics, we must thoroughly evaluate the thermal properties of the materials (see Table 3). With CONVERGE's CHT modeling, we can derive important data such as the thermal gradients within the solid regions and the development of the overall thermal profile. Figure 8 shows the predicted temperature at the liner-composite interface compared to the experiment, demonstrating that CONVERGE can capture the thermal behavior within the tank.

Part	Material	Density (kg/m^3)	Thermal conductivity ($W/m\text{-}K$)	Specific heat capacity ($J/kg\text{-}K$)
Injector	Stainless Steel	7990	500	16.2
Inlet and End Plug	Stainless Steel	7990	500	16.2
Inlet and End Boss	Aluminum	2730	167	900
Liner	Polymer	914	783	1799
Composite Wrapping	CFRP	1365	0.616	783

Table 3: *Properties of the different solid components.*

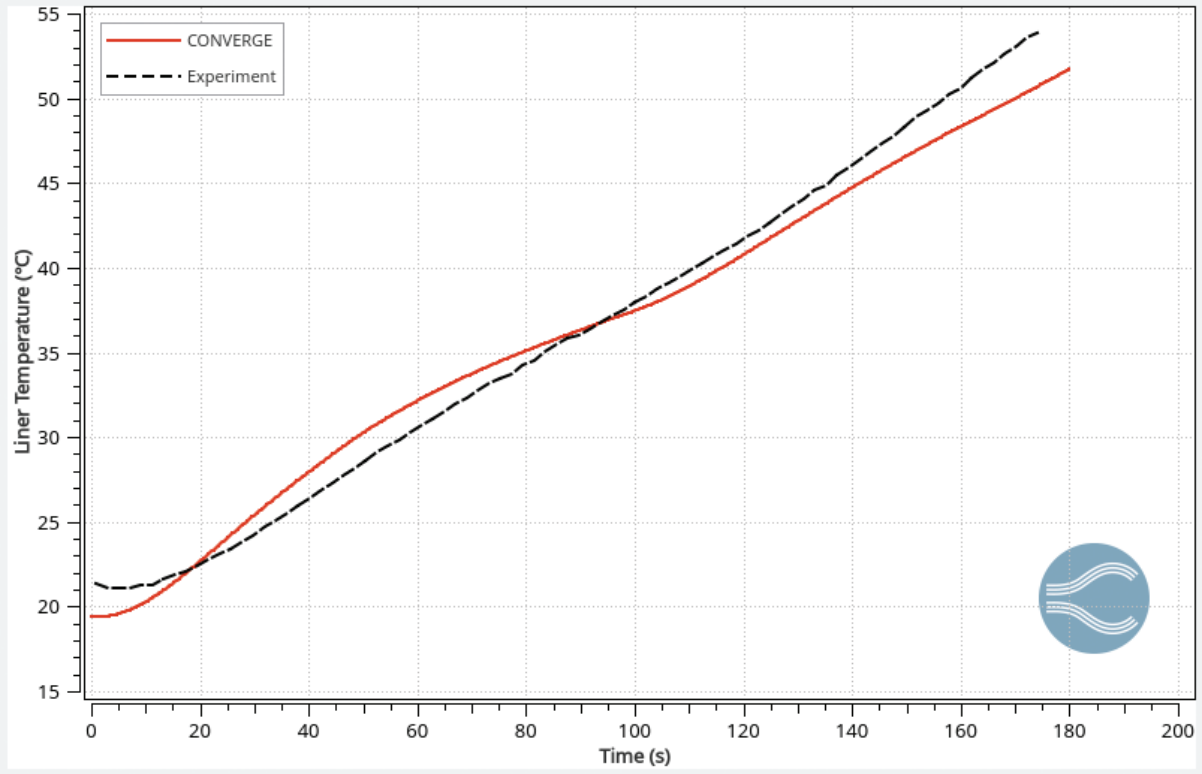


Figure 8: *Temperature evolution at the liner-composite interface.*

CONCLUSIONS

In this white paper, we discussed the major hurdles in hydrogen storage and highlighted the role of CFD as a tool for tank design and optimization. We demonstrated how CONVERGE can accurately and efficiently predict the hydrogen tank filling physics by simulating the filling scenario of a Hexagon 36L Type IV hydrogen tank from the HyTransfer EU project. For this study, we focused on the filling scenario through a 10 mm injector.

We compared the simulated flow dynamics and the thermal behavior during the filling process with experimental data,[1] which showed good agreement overall. We assessed major flow features, such as the pressure ramping during filling and the incoming jet dynamics, as well as the temperature profiles both qualitatively and quantitatively. The simulation allowed us to identify the recirculating vortical structures induced by the fluctuating behavior of the incoming jet. This phenomenon leads to the formation of hot gas pockets, which can affect the tank thermal distribution. The tank pressure measured at the rear location of the tank matched well with the experiment. The temperature profiles at the monitor locations inside the tank, accurately captured by CONVERGE, showed evidence of thermal stratification during the long filling process. Finally, we assessed the heat transfer across the tank shell by predicting the liner-composite interface temperature, which agreed well with the experimental data thanks to the CHT capabilities in CONVERGE.

The ease of use, flexibility, accuracy, and rich set of features make CONVERGE an effective tool for studying hydrogen tank filling (and emptying) physics and helping engineers improve their designs and technology.

If you want to learn more about how you can apply CONVERGE hydrogen technologies, visit our dedicated webpage, convergecfd.com/applications/hydrogen.

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Founded in Madison, Wisconsin, Convergent Science is a world leader in computational fluid dynamics (CFD) software. Its flagship product, CONVERGE, includes groundbreaking technology that eliminates the user-defined mesh, fully couples the automated mesh and the solver at runtime, and automatically refines the mesh when and where it is needed. CONVERGE is revolutionizing the CFD industry and shifting the paradigm toward predictive CFD.

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