PPS for Hydrogen Mobility

No Trouble with H_2

Fuel cells lend themselves to many areas in the transportation sector. Heavy-duty transportation in particular profits from the technology. However, the complex drive systems require special materials. Polyphenylene sulfide-based compounds developed specifically for this purpose not only offer the necessary mechanical and chemical resistance, but also greatly extend the systems' service life.

Fuel cell systems are particularly suitable for transport vehicles such as heavy-duty trucks.

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The ever-growing increase in CO_2 emissions caused, among other things, by fossil-energy use, has stimulated growth in renewable and eco-friendly energy solutions globally. Hydrogen is quickly becoming a global contender for alternative energy applications, and as such is attracting massive investments all over the world. Hydrogen is the most abundant element in the solar system, but on Earth it only occurs in compound form. Hydrogen must therefore be produced from molecules, being converted through specific processes such as thermo-chemical conversion, biochemical conversion, or water electrolysis.

Global hydrogen production today reaches about 75 million t per year, produced almost entirely from natural gas via steam gas reforming, and coal via coal gasification (grey hydrogen). Although hydrogen burns cleanly as a fuel at its point of use, producing it from fossil fuels without carbon capture only relocates emissions. Hence, to capitalize on hydrogen's full environmental benefits, it must be produced from zero carbon electricity through water electrolysis, an electrochemical process that splits water into hydrogen and oxygen (green hydrogen). Currently, however, water electrolysis accounts for less than 0.1 % of global hydrogen production. For this reason, many governments are also considering the temporary use of blue hydrogen, for which the released CO_2 is captured and then stored.

Cheap Green Hydrogen

Hydrogen's future global growth rate will be determined by two main factors: the competitiveness of its production costs and the availability of infrastructure. While the price of green hydrogen today is two to three times the price of grey hydrogen, economies of scale, government-driven carbon-pricing policies, and improved manufacturing processes will all reduce the cost delta and lead to more widespread green hydrogen use.

For decades, hydrogen has been primarily used by the chemical and refining industries in applications like the agricultural industry, the petroleum-refining industry, or in common industrial applications such as food, metalworking, welding, glass production, as a reducing and etching agent in electronics, or to create hydrogen peroxide in the medical industry. Newer hydrogen applications, like fuel cells or its use as a combustible fuel, open up new opportunities in transportation such as space exploration, aviation, heavy duty logistics, public transport, and even passenger cars. It is important to note, however, that these applications currently account for less than 10 % of global hydrogen consumption (**Fig. 1**).

High Pressure and Extreme Cold

Many of these new hydrogen applications operate under rather critical conditions at commercial scale. For example, the tanks which store hydrogen for fuel cell systems in a vehicle maintain pressures of 700 bar and above. Other liquid hydrogen applications operate at extreme cryogenic temperatures.

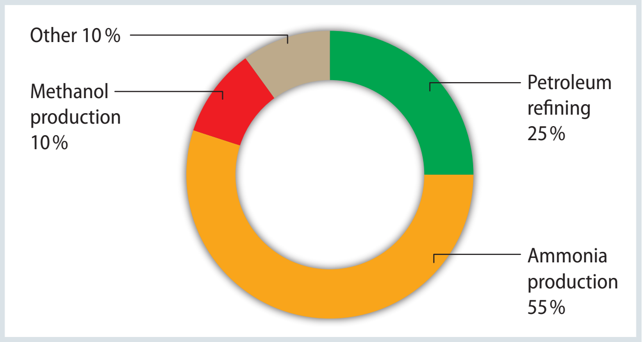

Fig. 1. Global hydrogen production by industry: The transport sector has played only a very minor role in this so far. Source: DSM based on Hydrogen Europe data; graphic: © Hanser

Using hydrogen as a fuel has many advantages:

- Infinite supply.
- Can be produced with zero carbon footprint from multiple sources.
- Easy to transport in large volumes.
- Produces clean power or heat at the point of use.
- Can be stored in large quantities for large time periods.

The supply of green hydrogen, however, presents a major hurdle to widespread hydrogen use. One critical technology in the production of low-emission hydrogen from renewable or nuclear electricity is electrolysis. The capacity for dedicated hydrogen production through electrolysis has recently been growing at an accelerated pace, driven by the growing demand for green hydrogen, and reached 8 GW per year in 2021. This increased to 13.6 GW in 2022, and is expected to grow to 21.4 GW in 2023 and 61.3 GW in 2030 [1]. Currently, Europe and China account for almost 85 % of total manufacturing capacity, but in the future, Australia and the US will see an increased contribution.

Many governments have significantly increased their ambition of increasing hydrogen capacity:

- In the US, the Bipartisan Infrastructure Law of the Biden administration includes grants for the creation of hydrogen hubs, and incentives to construct infrastructure for electrolysis manufacturing. The US DOE Loan Program Office has finalized a USD 504 million loan guarantee for a large-scale hydrogen storage project. The Inflation Reduction Act offers several tax credits as well as grant funding to support hydrogen technologies.
- In the EU, the Commission approved funding of EUR 5.4 billion to support its first hydrogen-related Important Project of Common European Interest with a focus on hydrogen technologies. Three more such projects, dealing with industrial applications, hydrogen infrastructure and mobility, are still to be launched in the near future.
- In Germany, the H2Global initiative has been launched, which uses a mechanism analogous to the CCfD (Carbon Contracts for Difference) approach to compensate the difference between supply prices (production and transport) and demand prices using grant funding from the German government.
- The UK presented a business model for low-carbon hydrogen for public consultation. The business model is based on a similar approach to CCfDs. The government aims to begin the first projects in 2023.

Hydrogen in Cars or Trucks?

Road transport contributes about 20 % of global CO_2 emissions from energy and 75 % of transportation-specific emissions. Most decarbonization efforts thus far have primarily focused on battery electric vehicles (BEV) for passenger cars and have resulted in great con-

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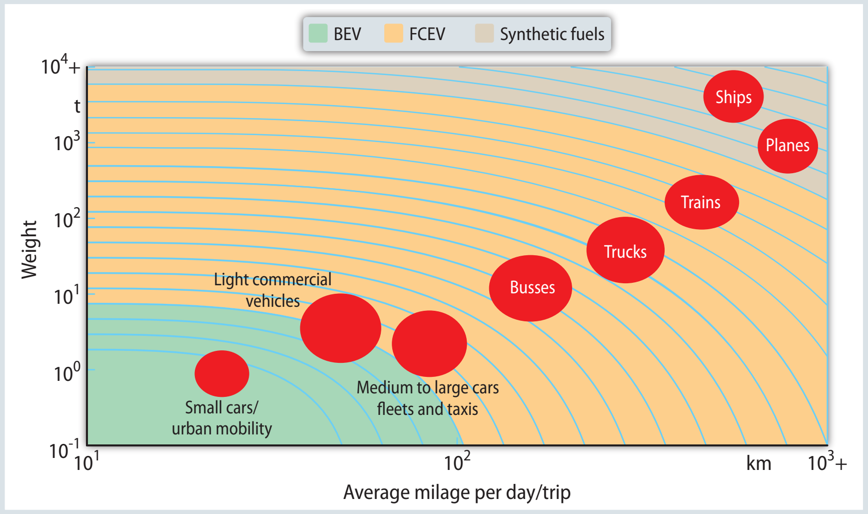

Fig. 2. Expected future distribution of drive types among the various transport sectors: electric vehicles will play a major role primarily in passenger cars, fuel cells more in transport vehicles.

Sources: Toyota, Hyundai, Daimler, Wiener Motorensymposium 2021; graphic: © Hanser

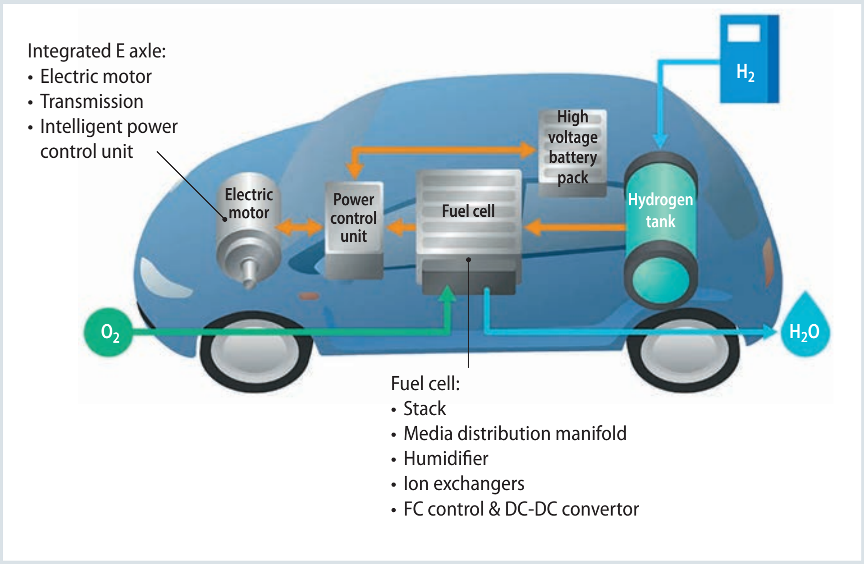

Fig. 3. Structure of a complete fuel cell powertrain. Source: Stock Images; graphic: © Hanser

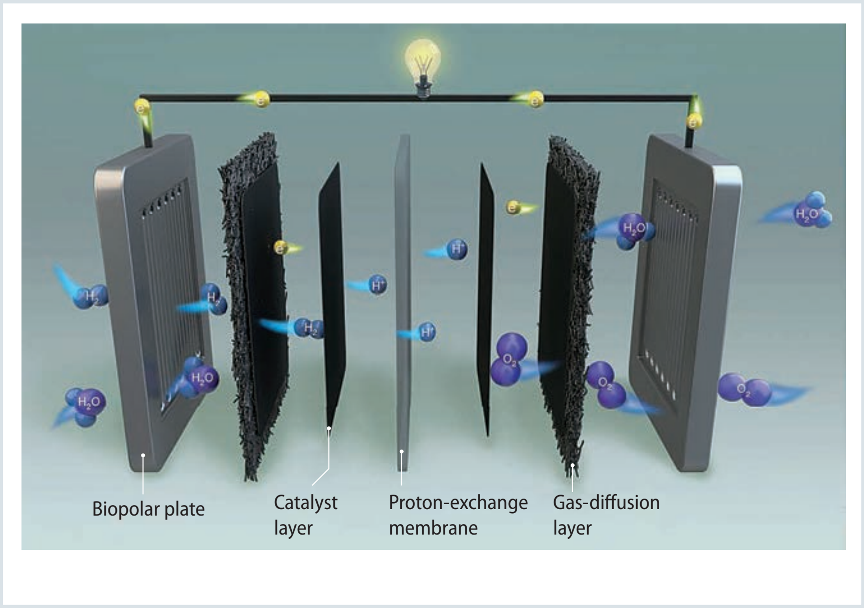

Fig. 4. Explosive view of stack individual cell: The choice of materials for the various components plays a very important role. Source: [4]; graphic: © Hanser

sumer response, with the BEV market reaching an all-time high in 2022. Heavy-duty applications, however, present a more challenging proposition for battery-electric technologies. There are more than 6 million heavy-duty trucks on the road in the EU alone, with a projected growth rate of more than 30 % by 2050. These vehicles require a vast amount of energy, and electrifying the whole heavy-duty fleet means massively increasing green electricity production in the EU. This green energy would also be fully dedicated to this purpose and could not be used in households or industry. With the EU's heavy-duty fleets' consumption of about 640 TWh of energy in 2020, the challenge to decarbonize road transport will be enormous.

While fuel cell electric vehicles (FCEVs) offer a big opportunity for the commercial sector, their widespread adoption faces issues which hinder widespread deployment. Due to their high cost, FCEVs are less competitive than BEVs or ICEs in terms of the total cost of ownership. This makes their economic fit less advantageous for the passenger car segment. The commercial segment, in which rapid fueling and high uptimes are required, is forecasted to be at cost parity by around 2025 for light-duty vehicles [2] and for heavy-duty diesel trucks by 2031 [3].

Hydrogen Combustion in Cars

Besides fuel cells, the heavy truck industry is also looking into hydrogen ICE (internal combustion engine) powertrains. A key drawback, however, remains that local NOx emissions continue to exist, and secondary SCR treatment of the combustion process may therefore be required. A shorter-term market introduction of hydrogen combustion-powered trucks may help to develop hydrogen fuel infrastructure, bridging the way forward for longer-term adoption of fuel cell trucks. In this way, hydrogen ICE and fuel cells are complementary technologies both driving the hydrogen economy forward. In this article, we will look closely at the long-term use of hydrogen in transport, zooming in primarily on the latest fuel cell technology and the related subject of hydrogen storage in high-pressure tanks.

Among different fuel cell variations, proton-exchange membrane fuel cell (PEMFC) technology is drawing significant attention in the transport sector – especially in commercial vehicles, which typically require more than 25,000 hours' operation time. Of the many component-level challenges, one of the most critical is selecting the right material for constructing components to meet the ever-increasing power density and endurance requirements of the fuel cell system. In this article, we present the latest development of material technologies from DSM Xytron PPS, which decrease ion leaching and total organic carbon (TOC), enable a more balanced mechanical performance and higher integration of the fuel cell system, and produce higher power densities and longer operational lifetimes.

Fuel Cell versus Electromobility

In the hydrogen economy, fuel cell vehicles (FCVs) are critical for delivering low-carbon transport. The well-to-wheels greenhouse gas emissions are expected to be reduced to near zero once hydrogen is produced from renewable sources, such as wind or solar panels. As the two low-carbon transport options – FCVs and BEVs

	DSM Xytron G4080HR (PPS-GF40)	Xytron G4080HRE (impact modified PPS-GF40)	PA66-GF35 (heat stabilized)	PPA6T-GF35	PA9T-GF30	PEEK-GF30	PPSU
Ion leaching (at 90 °C in distilled water)	+	+	–	○	○	+	+
TOC leaching	+	+	–	△	△	+	+
Mechanical retention (at 95 °C in hot water)	+	+	–	○	○	+	+
Mechanical retention (in hot water/glycol)	+	+	–	○	○	+	+
Glass transition temperature (dry state)	90 °C	90 °C	≈65 °C	≈147 °C	≈127 °C	≈155 °C	>180 °C
Glass transition temperature (at 90 °C in water)	90 °C	90 °C	<-10 °C	≈65 °C	≈70 °C	≈155 °C	>180 °C
Water absorption [weight %]	<0.5 %	<0.5 %	≈6.1 %	≈4.0 %	≈2.1 %	<0.5 %	<0.5 %
Dimensional stability (in FC working condition)	+	+	–	△	○	+	+
Mechanical creep resistance (in hot water)	+	+	–	△	△	+	○
Processability	+	+	–	△	○	△	△
Surface appearance (after molding)	+	+	–	△	○	△	+
Surface appearance (after long exposure in FC condition)	+	+	–	△	○	+	+
Electrical insulative properties (in FC condition)	+	+	–	○	○	+	+
Price	○	○	+	○	○	–	–

Performance indicator

– △ ○ +

Bad ⟶ Good

Table. Comparison of polymer compounds in fuell cell working conditions. Source: DSM

– are often compared. It is worth clarifying that batteries are energy storage devices, whereas fuel cells are energy conversion devices that typically use hydrogen for both energy storage and conversion. These two renewable transport options have some distinctive differences. BEVs outperform FCVs in energy efficiency, higher accessibility for charging infrastructure (both in public and private locations) and lower system costs.

Hydrogen offers multiple benefits when compared with both alternative fuels and BEVs in transport:

- Zero emissions when used in fuel cells and limited NOx emissions when used in ICE engines. This gives a distinct advantage compared with mineral oil-based fuels.
- Much shorter refueling times of about 3 min (comparable to gasoline refueling), which is a significant benefit where opportunity is limited for the long charge times of BEVs.
- Longer drive distances without the extra load of heavy batteries. A Class 8 heavy-duty truck would need up to a 1800 kwh battery pack to cover 500 km, which weighs up to 8 t.
- Much higher weather adaptability and much lower discharge capacity under sub-zero temperature conditions. Performance at –30°C is proven.

Those differences largely determine the application of each technical route. BEVs turn out to be a suitable alternative for passenger vehicles, while FCVs are more suitable for commercial vehicles (**Fig. 2**).

Well-Considered Selection of Material

A typical fuel-cell powertrain system consists of high-pressure hydrogen tanks (up to 700 bar), a fuel cell stack, an additional high voltage Li-ion battery pack, an integrated Eaxle, an integrated peripheric sub-system, such as a media distribution manifold, an integrated insulation plate, a water separator, a humidifier, an ion exchanger, valves, etc. (**Fig. 3**).

Unlike BEVs, which rely entirely on the power of Li-ion batteries, FCVs carry an electrochemical power generation system: the fuel cell (FC) stack, which converts hydrogen and oxygen into electricity (**Fig. 4**). Heat and water are the only by-products during this process. As the heart of the powertrain, the FC stack consists of hundreds of individual cells and various components made of plastic or metal. It is such a sophisticated device that external contamination, such as ion contamination or organic molecules, can severely jeopardize its durability and efficiency.

PEMFC systems operate in harsh conditions with temperatures ranging from 80 to 110 °C, in a mild to medium level of acidity, and fully humid conditions. Various materials, such as metal, rubber, and thermoplastics, are being utilized to build such fuel cell systems and engineering plastics are frequently selected due to their easy processability, light weight and intrinsic electrical insulation properties. There is a broad variety of engineering plastics that can be used for these applications.

Risks of Improper Material Selection

However, to build a fuel cell system for commercial vehicles that will survive long-term operation in these harsh working environments, proper engineering materials must be selected

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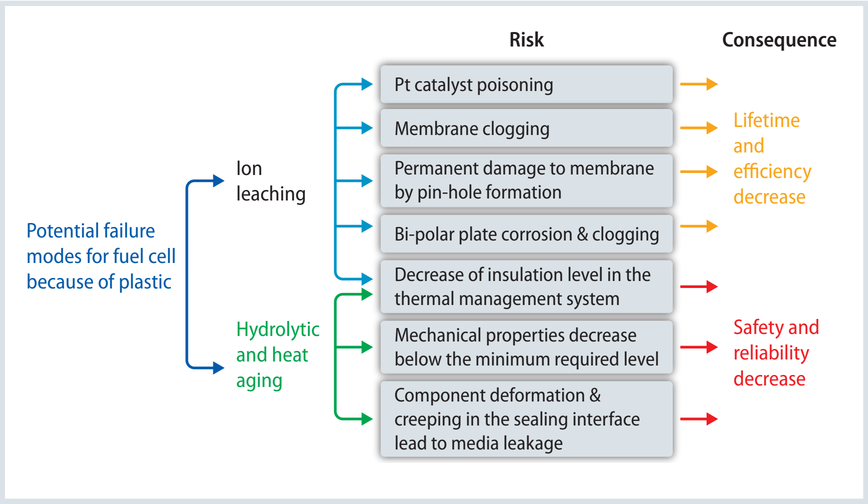


Fig. 5. Potential failure modes for a fuel cell because of an improper plastic selection. Especially the leaching of ions and the leaching of organic carbon molecules is a major problem.

Source: DSM; graphic: © Hanser

with careful regard for scientific and engineering precautions. These precautions must consider the need for very low ion and total organic carbon molecule leaching, excellent hydrolytic resistance, chemical resistance, mechanical creep resistance, and dimensional stability. Improper material selection could lead to catastrophic failures of the fuel cell (**Fig. 5**), including:

- Excessive ion leaching, anion poisons and cation ions, especially high valence metallic ions, show much higher affinity with sulfonic groups (-SO_3H) than proton does, which significantly reduces the power output of the stack. There are studies showing that even 5 ppm of Al^{3+} pollution in the membrane can cause total dysfunction of cell performance. The ranking for the metallic cations, from the perspective of their affinity to sulfonic group, is well studied by DSM as shown below:

  $\mathbf{Al^{3+} >> Ca^{2+} \sim Mg^{2+} > Ni^{2+} > Na^{+}, K^{+} > NH_4^{+}}$

  Ion leaching in the thermal management system also accelerates the corrosion of metallic bipolar plates and decreases the electrical insulation level of the vehicle.
- High amounts of total organic carbon molecule (TOC) leaching, which masks the catalyst and blocks the gas dispersion layer (GDL), leads to a significant reduction in the reactive catalyst's exposed surface and lower gas transmission efficiency.
- Part deformation, due to the hydrolytic degradation of material and reduction in mechanical creep resistance because of downshifting of the glass transition temperature (T_g): This mostly happens in polyamide (PA) compounds, which risk eventually leads to media leakage; thus, stack power output will be unstable and decreased.

Among various material solutions, PPS has been found to be the most suitable candidate. It combines the advantages of excellent chemical and hydrolytic resistance, low ion leaching, very good mechanical retention, and excellent electrical insulative properties in hot watery conditions. Thanks to its strong fundamental understanding of fuel cell poisoning mechanisms, DSM Engineering Materials has stepped into the future by developing a series of tailor-made PPS compounds with innovative interface technologies, not only suppressing the ion leaching of the compound, but also significantly improving long-term hydrolytic resistance. In addition, DSM has made a more mechanically balanced compound in the impact modifier Xytron G4080HRE, which improves ductility with minimum scarification on modulus and strength compared with the previous PPS GF40 compound, Xytron G4080HR. By combining these technologies, DSM's Xytron PPS compounds outperform alternative PPS compounds with very low ion leaching, super hydrolytic and chemical resistance, excellent mechanical creep resistance and more balanced mechanical properties (**Table**).

Prediction of Material Behavior

Through systematic scientific study, DSM has collected more than 10,000 material measurement data from fuel cell operation conditions. As a result, DSM has developed two major prediction models: the first calculates material mechanical retention in long term

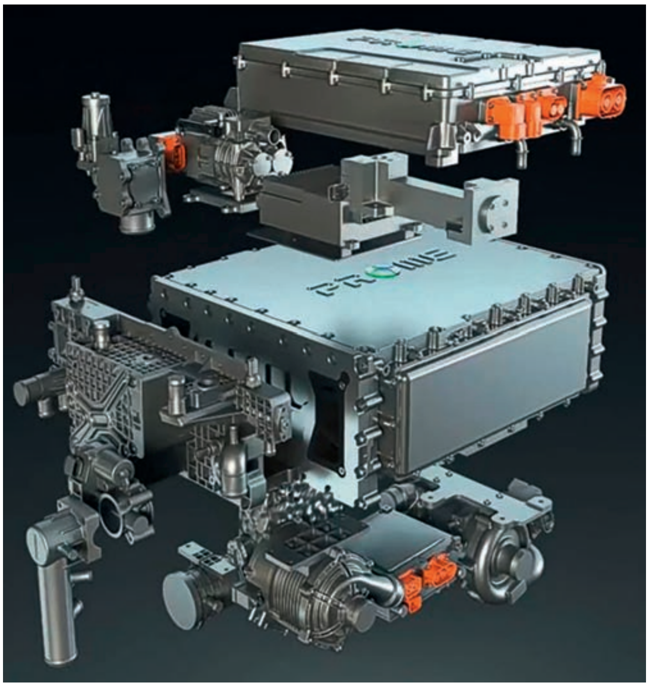
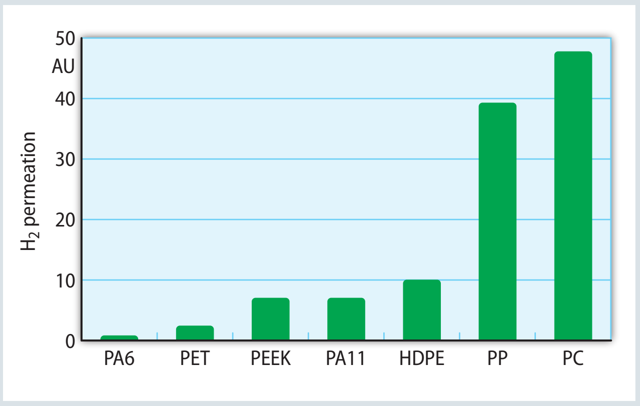


Fig. 6. For its fuel cell system SHPT Prome P4H, the Chinese manufacturer SHPT uses a PPS from DSM. © SHPT

Fig. 7. Hydrogen permeation performance of different materials. PA6 achieves the best values in comparison. Source: DSM; graphic: © Hanser



water/water glycol, enabling the precise prediction of material performance up to 80,000 h, and the second is a cell polarization curve prediction model, which predicts fuel cell efficiency against the influence of ion TOC leaching over time. This essential knowledge enabled DSM to significantly improve its fuel cell products. They out-perform other comparable polymers in terms of hydrolytic resistance, ion and TOC leaching, and long-term mechanical creep, fatigue and dimensional stability.

The developed PPS are already used by various companies for their fuel cell systems. For example, SHPT, a fuel cell powertrain manufacturer in China, chose Xytron G4080HRE for their latest fuel cell platform Prome P4H (**Fig. 6**).

Hydrogen storage is an important element of the hydrogen driving powertrain. It is well known that the energy density by weight (J/kg) of hydrogen is higher than that of regular gasoline, but because of its gaseous character at room temperature and ambient pressure, it is very low in energy density by volume.

The Difficulties of Hydrogen Storage

The industry has explored several options to overcome this challenge and ensure sufficient hydrogen in the vehicle to ensure a typical driving range comparable to a fully electric or gasoline/diesel equivalent vehicle. Consensus now seems to converge on the solution of compressing the hydrogen and storing it in a pressure vessel. To reduce the weight of the pressure vessel, a so-called type IV pressure vessel – made from a thermoplastic liner to govern the barrier properties, and carbon-fiber-based thermoset composite layer to withstand the high pressure – is preferred over steel or steel/aluminum/composite hybrids (type I–III). Both PA and polyethylene (PE) are considered polymer materials in the manufacture of such liners. Within the PA family, the most frequently considered materials are PA6- and PA11-based compounds.

PA6, PA11 or PE?

From a purely permeation-based point of view, PA6 is superior in intrinsic permeation behavior compared with HDPE (factor 10) and PA11 (factor 7) (**Fig. 7**). The intrinsic permeation behavior of impact-modified PA6-based compounds, such as the Akulon Fuel Lock materials, is still significantly better in barrier performance compared with PA11 and HDPE. Analyses of permeation behavior with molecular simulations showed that the difference scales with the solubility of the hydrogen in the polymer materials, and that solubility scales with the concentration or density of amide bonds (or absence thereof, in the case of HDPE) in the polymer chains.

Summary

The production and use of green hydrogen provide a new possibility of zero-emission energy and the lowest possible environmental impact, which contributes to a carbon-neutral society. PEMFC can be one of the answers to greenhouse gas emissions for the transport sector. The application of PEMFC is not limited to the automotive sector, but can be applied to forklifts, airplanes, trains, boats, and drones. Alongside green hydrogen production and storage, this forms a technology platform with vast possibilities – and many countries around the world are advancing their ambitious hydrogen plans.

To embrace this new era, DSM scientists have been working to build their fundamental understanding of the hydrogen industry. As a result of their work, DSM has tailor-made the Xytron PPS fuel cell platform, along with its Akulon Fuel Lock portfolio, to store hydrogen at high pressures. The aim is to support the development of reliable fuel cell powertrains for commercial transport and hydrogen production from PEM electrolyzers. DSM's Xytron PPS platform provides products with a balanced mechanical performance, very long ion and TOC leaching, super hydrolytic resistance, super mechanical creep and fatigue performance after aging, and excellent electrical insulative properties in FC operational conditions. Akulon Fuel Lock provides the lowest hydrogen permeation of all tested materials while delivering excellent mechanical and low-temperature-burst performance. With both material solutions together, the entire hydrogen system in transport applications is covered. ■

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