Accelerating the Hydrogen Economy Through Digitalization

by Ron Beck, Industry Marketing Senior Director, Aspen Technology Inc.

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Introduction

The energy transition, coupled with a global drive for sustainability in the energy and chemical industries, is already impacting the economy and all players across the energy value chain. These geopolitical forces will create winners and losers across these industries over the next 10 years.

Renewable energy such as wind and solar power generation are of unequal potential geographically. Many parts of Asia are challenged by limited access to locations that can generate substantial solar or wind power. (See Figure 1.) In addition, liquid fuels are difficult to substitute in several applications such as air and ocean transport.

What's more, electrification of vehicles and other applications will create a large future demand for metals processing, which has an uncertain lifecycle carbon impact.

Enter hydrogen. Hydrogen offers the opportunity to fill a significant fraction of the world's need for energy and can be generated carbon-free. However, hydrogen also presents several challenges, especially with respect to storage, transport, cost of electrolysis generation, sources and availability of renewable electricity for electrolysis, cost and efficiency of carbon capture (in the case of blue hydrogen) and safety. The race is on to reduce the cost penalty of utilizing hydrogen in comparison with other energy sources (coined "Green Premium" by Bill Gates in 2020).

Despite these challenges, the hydrogen economy is seeing strong momentum reflected in announced capital projects that aim to deliver hydrogen generation and storage at scale. In fact, several regions are investigating the feasibility of a hydrogen economy as a significant zero-carbon alternative.

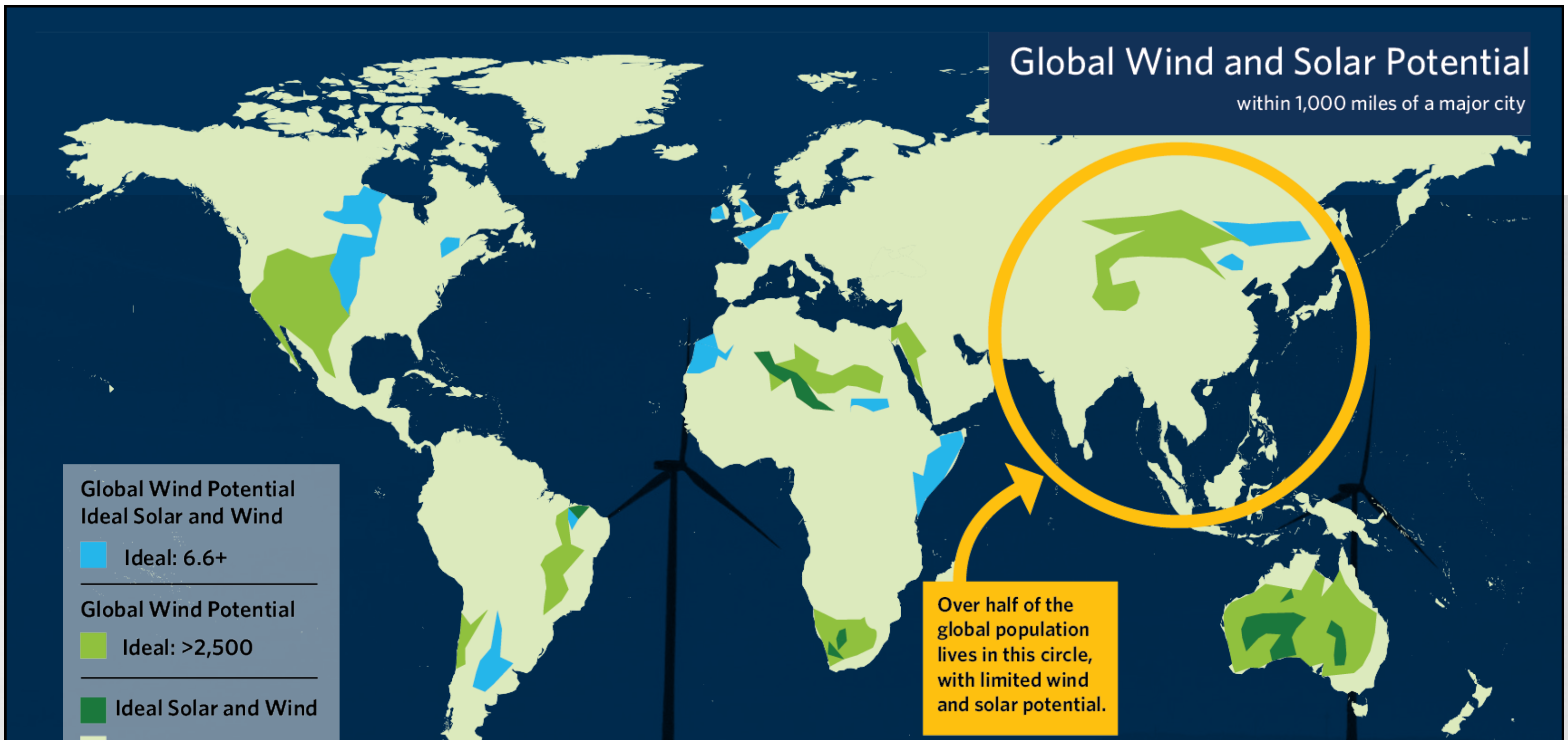


Figure 1: Global wind and solar energy potential. (Source: Peter Ziehan)

Digital technology will be an essential component in delivering the hydrogen economy, accelerating and de-risking innovation, de-risking adoption and enabling faster and better scale-up and optimization of the hydrogen value chain. It will be fundamental in overcoming many value chain obstacles, maximizing commercialization, design and supply chains, and boosting production and economics.

> "The sustainability revolution will be powered by digital technology."
>
> *- Al Gore, Chairman, Generation Investment Management, January 22, 2021, Davos*

Which digital technologies will be most important? Developing hydrogen as an energy source involves the complete value chain from production to end-use—and encompasses the entire commercialization lifecycle, from innovation to reliable operation at scale. Innovations in asset optimization software now span design, operations, supply chain and maintenance, and are uniquely suited to address these challenges.

These solutions incorporate modeling of hydrogen and carbon capture processes, risk and availability assessment across the value chain, incorporating stochastic modeling and asset health monitoring. (See Figure 2.)

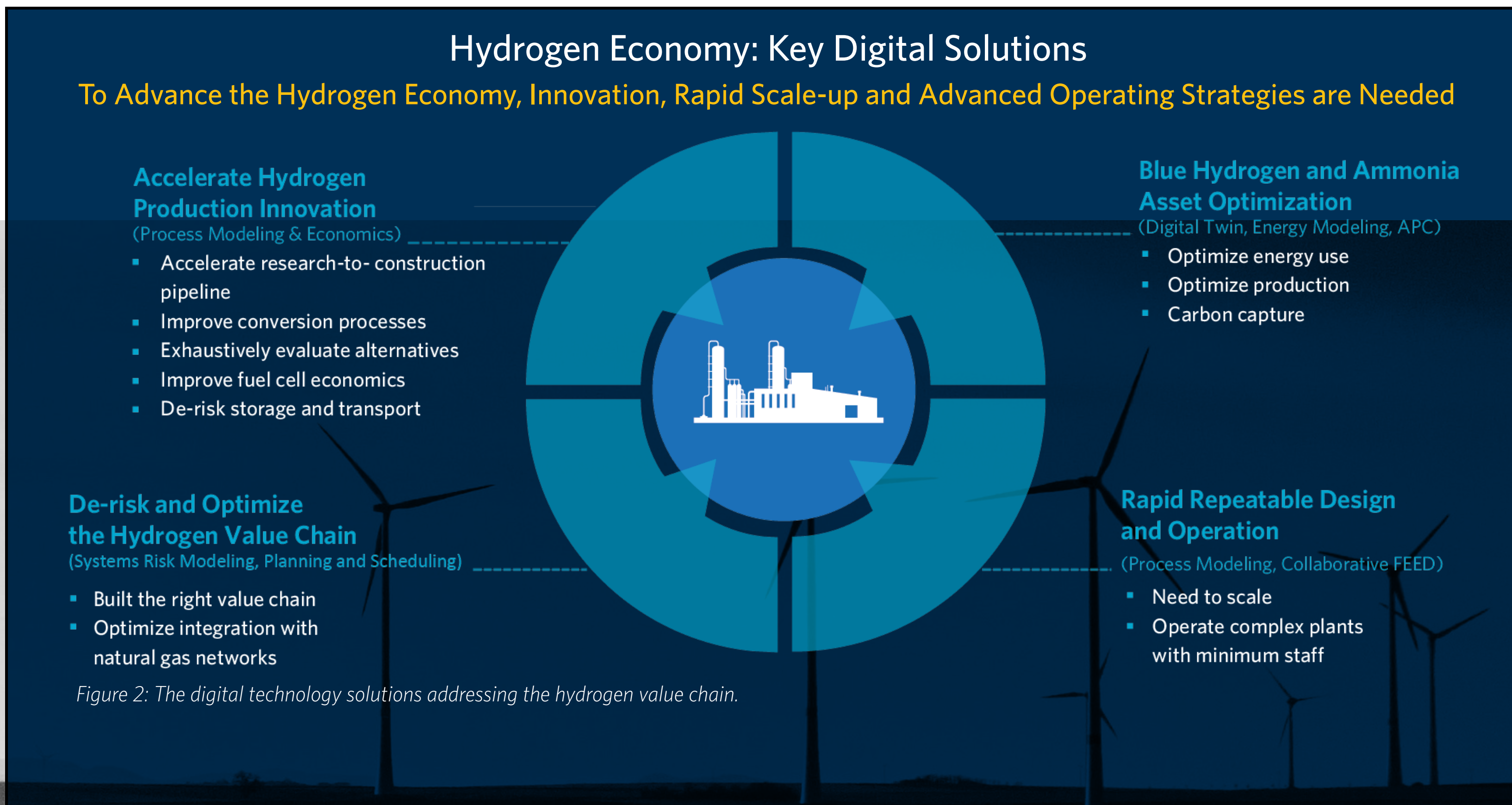


Figure 2: The digital technology solutions addressing the hydrogen value chain.

The Role of Digital Technology in Hydrogen

Simply put, software technology will be a strategic asset as the industry seeks to successfully navigate the energy transition. In the case of the hydrogen economy, digital technology will be a major accelerator for driving down the cost of hydrogen, evaluating and optimizing many value chain alternatives and removing constraints to safely scale the value chain.

Drilling down further, here's how today's digital technologies can expedite the transition to hydrogen, impacting key functional areas:

- **Employing advanced methods for innovation and optioneering, while driving down costs.** Rigorous process simulation software can represent hydrogen electrolysis, hydrogen reformer processes, other innovative hydrogen synthesis approaches and hydrogen liquefaction and pipeline transport—accelerating commercialization and improving access to capital.[1]

  Several specific digital technology opportunities to accelerate innovation include:

  - Hybrid models incorporating Artificial Intelligence (AI) together with first principles models for new processes, including membrane technology, combining reforming, carbon capture and novel processes
  - Rate-based simulation modeling for carbon capture
  - Powerful, rigorous models to handle electrochemistry
  - High-performance computing for evaluating thousands of alternatives in an optioneering context
  - Integrated economics to rapidly screen techno-economic alternatives during concept design and pilot plant testing

- **Integrating collaborative engineering workflows.** Cross-functional teams will be able to rapidly select concepts, scale-up designs, execute projects and use modular design to accelerate industrial implementation. This will drive down project timetables 50 percent or more.[2]

- **Facilitating advanced, integrated supply chain planning.** New software advances optimally integrate the hydrogen economy value chain with existing natural gas and power networks.

- **Automating processes to create the self-optimizing plant paradigm.** New technologies such as hydrogen electrolysis, carbon capture, crude to chemicals and industrial scale fuel cells to be deployed as autonomously as possible to compensate for shortages of highly skilled operators.[3]

- **Optimizing the value chain with risk and availability modeling.** Use new capabilities to evaluate hydrogen production, transportation, storage and end-use options as well as the risks to achieve reliable energy goals.

For both hydrogen electrolysis and fuel cells, the ability to simulate electrochemistry, handle dynamics and consider stochastic variation are all crucial. Advanced modeling and digital twin solutions have played a prominent role in the hydrogen generation research and development arena for the past 30 years, from electrolysis and steam reforming to carbon capture and fuel cells. The rigor, accuracy and flexibility of AspenTech modeling technologies have made them a preferred choice for industrial and government research, as well as academic initiatives related to hydrogen and carbon capture.

Aspen Plus® is a proven modeling solution for applications such as fuel cells and hydrogen electrolysis processes due to its ability to rigorously model complex chemical processes and effectively model the electrochemistry. The ability to rapidly estimate economics also makes this a strategic tool for techno-economic analysis.

Hydrogen Challenges: Scale-up, Distribution and Reliability

To accelerate hydrogen production while achieving favorable economics, the industry will need to focus on several areas including: (1) conversion efficiency, process optimization and scale-up of hydrogen production—including selection of the most advantageous production approach that will drive down production costs; (2) development of low-cost and efficient hydrogen distribution and storage value chains, including evaluation of carrier alternatives such as ammonia and cryogenic and solid hydrogen; and (3) implementation of low-risk, high-reliability and cost-competitive hydrogen end-user technology.

Central challenges for green and blue hydrogen production include the identification and rapid evaluation of highest efficiency electrolysis and/or membrane conversion approaches, evaluation of economics of catalyst and adsorbent options, and improvement of economics based on highest cost choke points.

Figure 3 below summarizes a simplified state of play of the basic options (of course, it is more complicated than this as carbon capture must be combined with blue hydrogen synthesis). Within the framework outlined, several key alternatives include:

Hydrogen Production: Ways to Commercialize Clean Hydrogen

	Process	Pros	Cons	Maturity	Efficiency (%)	Costs relative to SMR	Aspen +, HYSYS Models
Blue and Grey Hydrogen	Steam methane reforming (SMR)	Best H to C ratio	CO2 emission	Mature	70-85	1 [1]	Both
	Partial oxidation	No catalyst	CO2 emission	Mature	60-75	1.8 [1]	Both
	Autothermal reforming		CO2 emission	R&D	60-75	1	Both
	Naphtha reforming		H2 is by product	Mature		1	Both
CCU	Carbon capture (necessary aspect of blue hydrogen)	Know technology	High energy penalty	Early commercial	N.A.	N.A.	Both
Brown H2	Coal gasification	Large scale, low cost	Large CO2 emission	Mature	60	1.4-2.6 [1]	Aspen+
Green Hydrogen	Biomass gasification	Carbon neutral	Low efficiency	R&D	35-50	2.0-2.4	Aspen+
	Electrolysis of water	CO2, scalable	Expensive	Mature	10-50	3-10	Both plus ACM
	Wind/Solar assist electrolysis of water	CO2 free	System needs to be optimized	R&D			Both plus ACM
	Photobiological, photoelectron-chemical, thin-film solar	CO2 free	Technology not proven	R&D	Potentially >50		Aspen+, ACM

[1] Not including CO_2 capture costs

Figure 3: Main hydrogen production technology options, economic strengths/weaknesses and, in the last column, the main modeling systems used to design and optimize these options.

1. Distributed hydrogen production modules versus large centralized production.
2. A phased approach, leveraging both blue and green hydrogen options initially and migrating to higher efficiency green hydrogen as economics improve over time and technical risk diminishes.
3. R&D to drive down the cost of fuel cells for end-use, electrolysis for production and to reduce risk in transport and storage.
4. Focus on larger scale, concentrated end-uses such as power generation and grid storage in the shorter term.

Solution: Digitalization Across the Value Chain

As the industry transitions to hydrogen, it's vital that companies look for asset optimization software that extends across the entire value chain, addressing the key areas of Production, Distribution and Storage and Usage. (See Figure 4.)

Here's a closer look at how today's digital solutions can assist companies as they explore all avenues of the hydrogen economy.

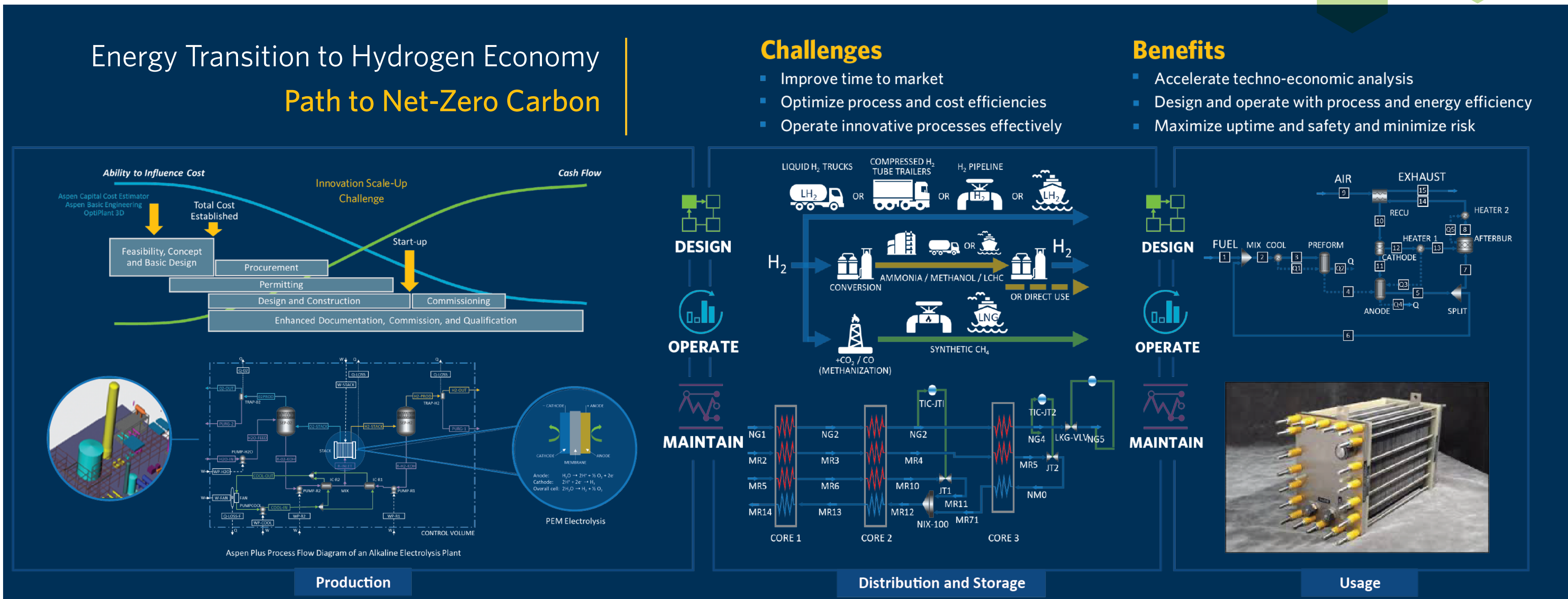


Figure 4: Addressing the hydrogen value chain with one set of digital solutions.

Selecting Green or Blue Technology—A System Solution

The hydrogen economy offers many aternatives and permutations. The most appropriate choice of technologies will be highly dependent on regional energy options, industrial players and government policies. Currently, industry participants from Europe and the Middle East to APAC and Latin America are pursuing different pathways to the same end goal.

To effectively understand the alternatives, economics and risks, a comprehensive view of systems risk is crucial, especially when assessing the impacts to the proposed value chains. This is where a system risk analysis tool like Aspen Fidelis™ is ideal as it includes a built-in, pro forma hydrogen economy model to facilitate these analyses. (See Figure 5.)

Innovation and Conceptual Design

Green Hydrogen Electrolysis. Advances in today's custom unit modeling technology can uniquely handle electrochemistry, including electrolyte properties and power-to-model electrolysis, end-to-end. Gas and chemical providers like **Air Products** and **Air Liquide** are currently leveraging solutions that push the modeling frontiers with respect to electrolysis reactors for hydrogen production.

Blue Hydrogen—Reforming. Best-in-class engineering software models and optimizes process routes and energy use in producing hydrogen from natural gas or from coal. Air Products, a leader in both blue and green hydrogen that effectively performs carbon capture today, recently presented a case study on its hydrogen modeling for optimizing installed hydrogen plants to deploy blue hydrogen.

Carbon Capture. Carbon capture is receiving increasing investment attention within the industry. As hydrocarbons and metals continue to be in demand in the global energy and resource mix, CO_2 will continue to be a byproduct of conversion. Carbon capture, using a variety of technology alternatives, is racing toward broader commercial viability. The main challenges include minimizing energy use during CO_2 capture, optimizing CO_2 capture processes in the face

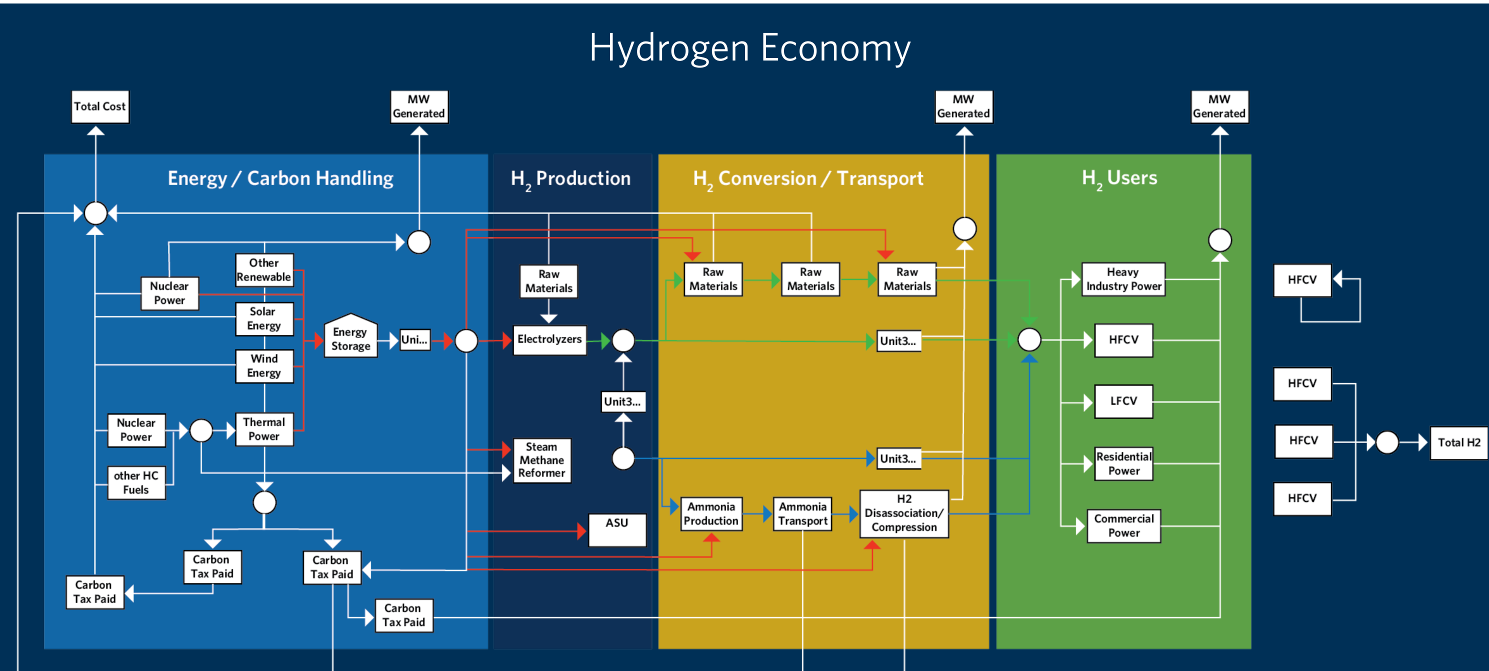


Figure 5: Modeling the end-to-end hydrogen economy value chain in Aspen Fidelis; enables view of optimal investment strategies to minimize risk and maximize economics and energy availability.

of complex chemistry and effectively maximizing the recharge and reuse of catalyst and adsorbent materials to avoid creating a secondary waste disposal challenge.

Advanced process modeling is a vital element when solving these technical challenges and improving economics, as well as when ensuring operational integrity, energy optimization and improvement. Companies need to look for highly differentiated, rate-based modeling—the most rigorous, accurate and efficient method for modeling solvent-based carbon capture processes. Additionally, custom unit modeling as well as AI-based hybrid models can be used to model the advanced membrane technologies currently being tested for carbon capture.

Leaders in the carbon capture arena using digital tools to make their innovative leaps include most universities performing work in that area, several government research labs and research centers such as **US NETL, MIT Energy Center, US EERC and Canada CANMET.** There are also key commercial players in carbon capture such as **Cansolv** (Shell technology group for carbon capture chemicals), Dow, Fluor (who has carbon capture technology), **Carbon Capture Inc., Carbon Engineering, Technology Centre Mongstad** and others. Several refiners and chemical producers are also employing chemical and energy simulation software to model end-to-end carbon capture. (See Figure 6 for digital solutions that create value in the carbon capture process.)

Hydrogen Liquefaction and Storage. A strong modeling environment can predict the performance and safety of hydrogen liquefaction designs. The **Norwegian NTNU** (Norwegian University of Science and Technology), for example, has demonstrated how liquefaction can be rigorously modeled in tools like Aspen HYSYS®.

Fuel Cell Technology. As with electrolysis, today's digital applications have unique power and flexibility to model and improve fuel cell technology. In this case, areas such as adsorption modeling and dynamic modeling are also crucial elements to look for in these tools. Several dozen players in fuel cells are using these technologies to their advantage including

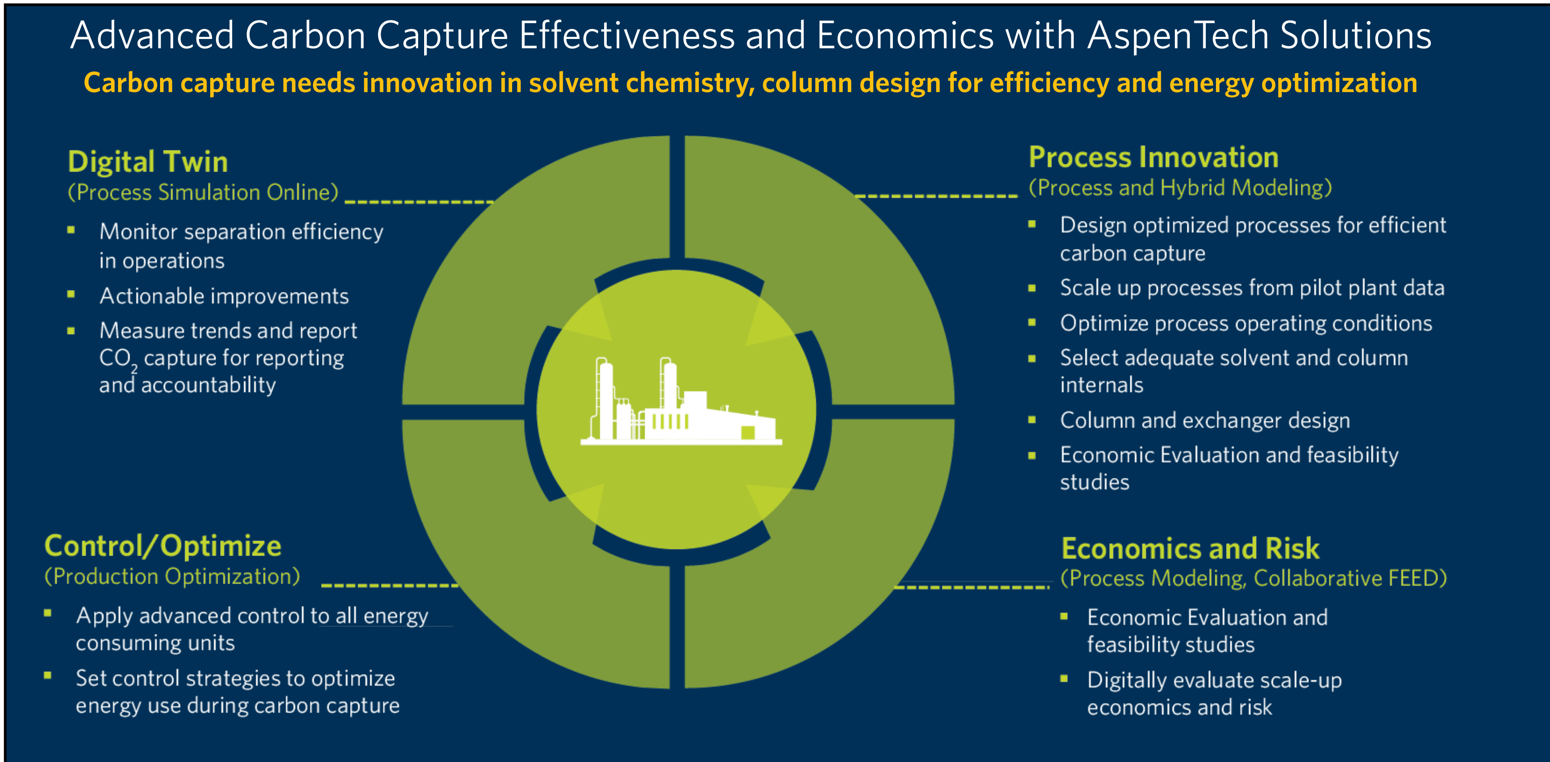


Figure 6: Key digital solution areas to drive carbon capture costs down.

Fuel Cell Energy Inc., which makes distributed industrial fuel cell units, and Doosan in Korea. (See Figure 7 for an example of a fuel cell system model.)

Optioneering and Commercialization

Today's digital solutions provide integrated workflows that provide powerful innovation capability during R&D, conceptual design, techno-economic optioneering and commercialization. These advanced tools are already proving crucial in driving down the cost of hydrogen, improving economics and executing at scale. Key differentiators to look for include:

Optioneering workflows to rapidly find the optimal technology and execution from a cost, sustainability and reliability view:

- High-performance computing and integration solutions rapidly screen thousands of process alternatives and identify the leading candidates, crucial in areas like green hydrogen and carbon capture where the optimal process designs are still under development.
- Companies can also leverage integrated economic and cost modeling, energy efficiency optimization and risk modeling workflows to explore cost and energy sensitivity of different alternatives. These tools are being used by ERTC, Technology Center Mongstad, NETL and others to conduct techno-economic evaluation during concept development.

Conceptual layout workflow:

- Conceptual 3D layout software tied to process simulation optimizes fitting process designs into constraints of either existing or new plant sites, and in the case of distributed implementation, fits a fuel cell unit or hydrogen production unit into an existing site like a power or fueling station. This approach has been adopted by ExxonMobil to reuse asset 3D models during conceptual design.

Modular design workflow:

- A range of modular design tools rapidly develops reusable and reconfigurable designs that can be used for distributed hydrogen production, industrial fuel cell or carbon capture—and achieves the scope and scale that a company's strategy will require.

Hydrogen End Use

Digital technology addressing fuel call challenges and creating value

Challenges

- Design and commercialize fuel cell
- Operate power systems effectively
- End use safety and waste heat management

Benefits

- Design of cost-effective fuel cells for safe hydrogen use
- Optimized operation of integrated power systems
- Efficient cogeneration and heat and electricity management

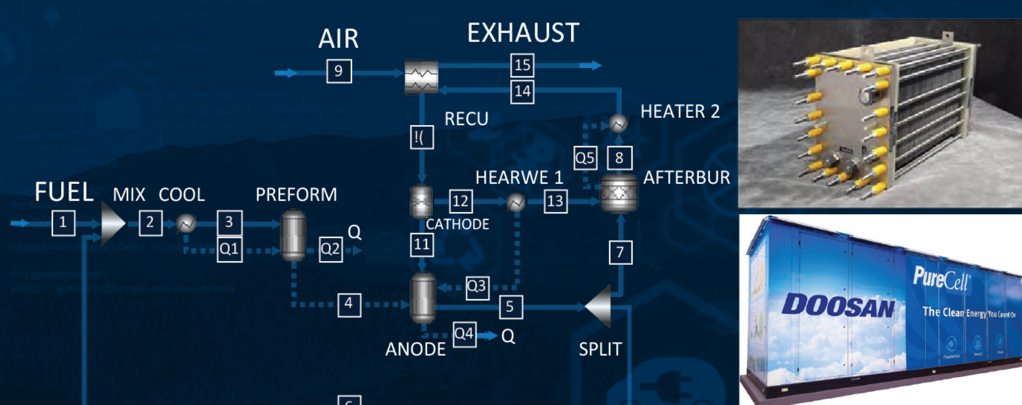


Figure 7: Example of fuel cell modeling for design and optimization demonstrating safety, efficiency and economic benefits.

Industrial AI-powered workflow:

- Accelerate the discovery of opportunities much faster when you can build models from lab and bench data (hybrid models) and leverage AI to identify strategies for implementing and debottlenecking hydrogen distribution supply chains.

Advanced Control and Optimization

Best-in-class adaptive process control and dynamic optimization technology will be crucial in the control and reliability of new and complex technologies represented by hydrogen production and carbon capture. Many refiners use adaptive process control on their existing hydrogen plants and are leading the implementation of dynamic optimization, which has significantly reduced energy use, hydrogen loss and flaring at sites like CEPSA RLR Refinery's hydrogen network.

Integrated Supply Chain

The hydrogen economy will require an evolutionary approach to migrating existing energy distribution supply chains into one that will evolve to handle grey, blue and green hydrogen. Today's advanced planning, scheduling and supply chain tools provide energy companies like Bold Reliance a unified platform to handle the end-to-end supply chain across businesses in a unique way. Additionally, enterprise risk modeling systems will be crucial in understanding success factors in supply chain implementation.

Beyond Hydrogen: Short- and Long-Term Sustainability

The energy industry today is facing a number of challenges—the need to drive to net-zero carbon, macroeconomics impacting global demand for hydrocarbons and an energy transition that's gaining momentum and building demand for renewable electricity and zero-carbon mobility solutions.

At the World Economic Forum's Davos Agenda in January 2021, Bill Gates talked about the need to create a trusted global carbon market, which will spur the need to shift very large capital investments into low carbon areas. He talked specifically about the hydrogen economy, carbon capture and energy storage, as well as Green Premiums and driving the economics of new technologies through scaling and investment.

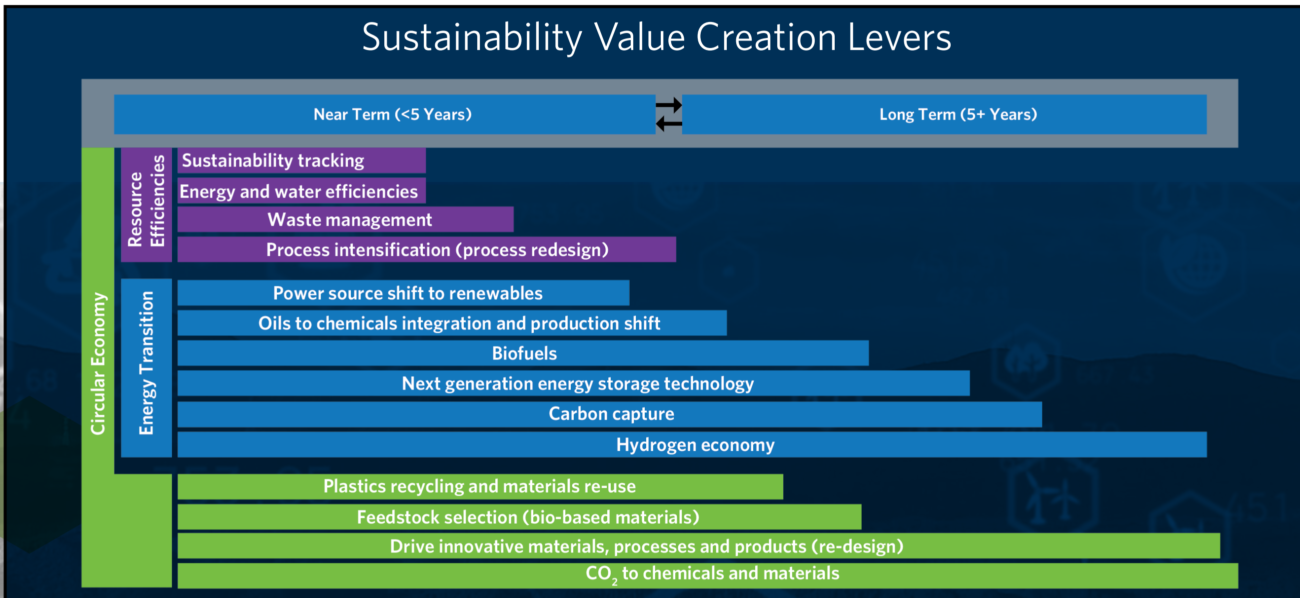


Figure 8: Key sustainability levers for energy and chemical companies.

There are unique and differentiated technologies available today with respect to innovating, scaling and achieving competitive advantage in the hydrogen economy, biofuels and other energy transition strategies.

Figure 8 summarizes the value creation levers that the process industry is expected to employ to proactively drive decarbonization and energy transition. Additionally, hydrogen provides an energy source for circular economy programs that seek to eliminate emissions and waste in production.

There is significant opportunity now for companies to accelerate the time-to-value for the hydrogen economy, carbon capture and biofuels by leveraging today's digital solutions that help ensure faster adoption, scale and competitive advantage.

Technology Solutions to Jumpstart Sustainability

The extent of the energy transition complexity requires a balance of the many objectives across a company's assets and a data-based and quantitative approach. Digitalization and Industrial AI will be crucial tools in this balancing act. Al Gore stated at the WEF Davos Agenda in January 2021, "The sustainability revolution will be powered by digital technology." Figure 9 demonstrates how digital technologies map closely to the essential elements of the energy transition that the industry is considering.

Sustainability Use Cases Enabled by Technology Solution Sets

		Resource Efficiency		Energy Transition					Circular Economy			
		Emissions (all GHG Sources)	Energy & Water Efficiency	Biofuels	Carbon Capture & Utilization	Green & Blue Hydrogen	Crude to Chemicals	Solar/Wind /ÞRenewable /ÞStorage	Plastics and Materials Recycling	CO$_2$ to Chemicals	Innovative Process/ Products	Bio-Based Feedstock
All	Energy and Emissions Monitoring/Optimization	Major impact	Major impact	Major impact	Major impact	Major impact	Major impact		Major impact	Major impact	Major impact	Major impact
Performance Eng.	Strategy, Capital Planning (CAPEX) and Design	Supporting role	Supporting role	Major impact	Major impact	Major impact	Major impact		Major impact	Major impact	Major impact	Major impact
Performance Eng.	Digital Twin	Major impact	Major impact	Supporting role	Major impact	Major impact	Major impact		Major impact	Major impact	Major impact	Major impact
Performance Eng.	Utility Optimization	Supporting role	Major impact			Supporting role	Major impact	Major impact	Major impact	Major impact	Major impact	
Prod. Opt.	Planning & Schedule		Major impact	Supporting role	Supporting role	Supporting role	Major impact		Supporting role		Supporting role	Supporting role
Prod. Opt.	Control & Optimize	Supporting role	Major impact	Major impact	Major impact	Major impact	Major impact		Major impact	Major impact	Major impact	Major impact
Prod. Opt.	Monitor & Execute	Major impact		Major impact	Major impact	Supporting role	Supporting role	Major impact	Supporting role	Supporting role	Major impact	Major impact
Value Chain	Supply/Value Chain Optimization			Supporting role	Supporting role	Major impact	Major impact		Major impact	Supporting role	Supporting role	Supporting role
Value Chain	Waste Accounting	Major impact	Supporting role	Major impact			Supporting role		Supporting role	Supporting role	Supporting role	Supporting role
APM	Predictive Maintenance and Asset Health	Major impact			Supporting role	Supporting role	Major impact	Major impact	Supporting role	Supporting role	Supporting role	Supporting role

Major impact   Supporting role

Figure 9: AspenTech solutions that strategically create value for sustainability use cases.

Examples of publicly disclosed case studies of sustainability value created by digital technology are summarized in Figure 10.

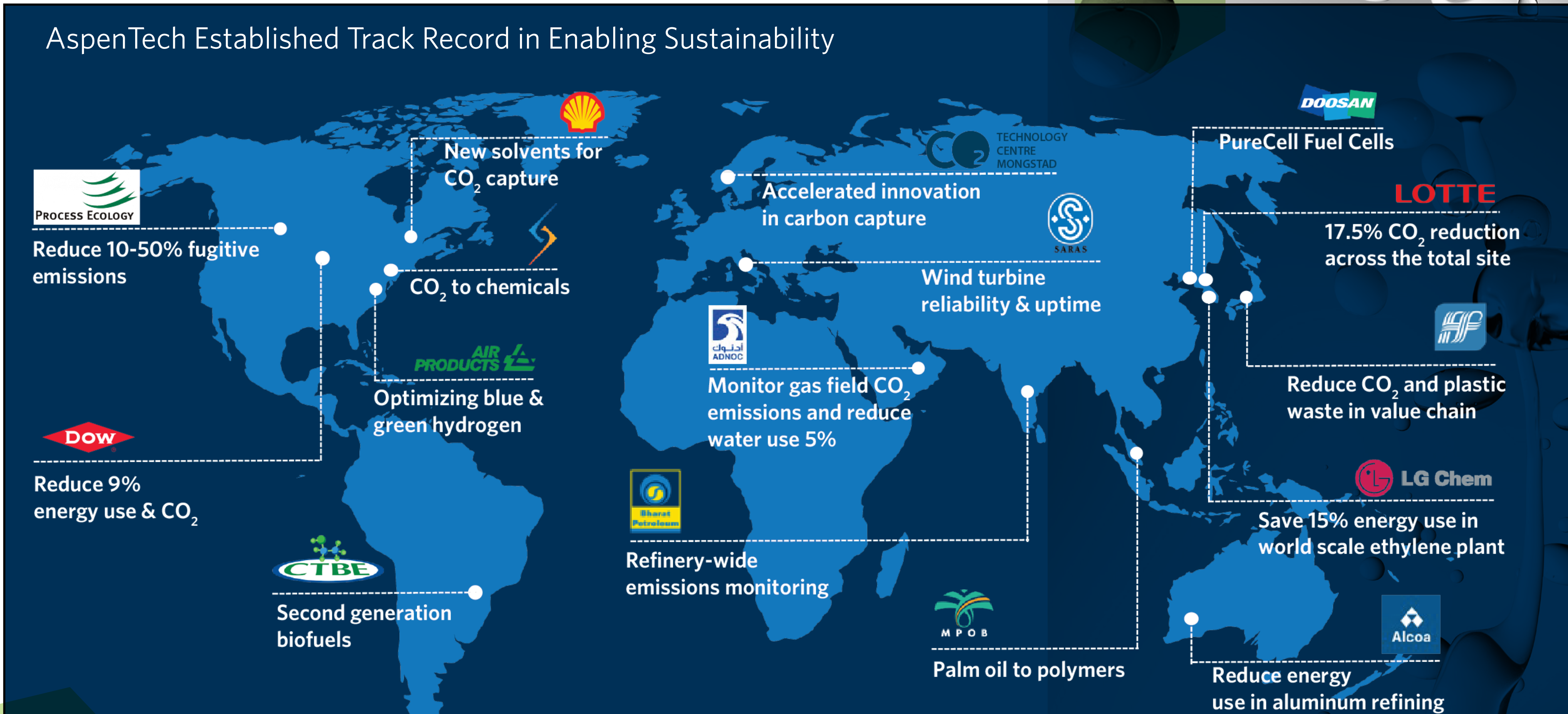


Figure 10: Examples of sustainability value created by AspenTech technology solutions.

Conclusion

Why Partner with AspenTech Now?
The current macro-economic pivot toward sustainability and energy transition, and the momentum behind it, make it especially attractive today for industry and technology players to work more closely and collaboratively than ever before. Innovative ideas from both sides can achieve unprecedented breakthroughs.

Achieving energy transition leadership with industrial-scale hydrogen production and carbon capture technologies will require an unmatched level of innovation, creativity, agility and execution. This is a clear area where a software technology innovator like AspenTech can complement and add value to industry participants, individually and collectively.

Areas where shareholder value is created from the use of technology include:

- **Time to market:** Accelerating innovation, optioneering, concept selection and capital investment decision-making by up to 50 percent (or six to 12 months).

- **Cost of production:** Reduce capital cost through visual estimating, reduce operating costs by saving energy and water through optimized designs, and incorporating new technology effectively into existing facilities.

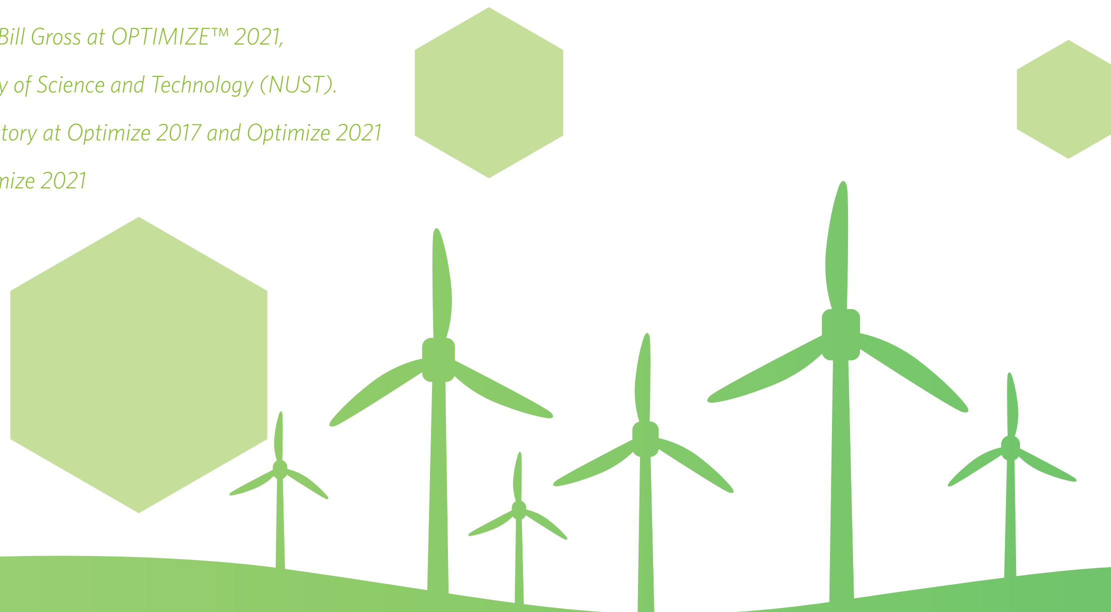
- **Uptime, Safety and Risk:** Employ AI and analytics to reduce risk while improving uptime, safety and reliability.

- **Customer satisfaction:** Maximize agility and resilience in the supply chain.

As you look to navigate your own transition and consider the technologies that will best align with your requirements, we invite you to learn more about the viable, proven solutions from AspenTech.

Citations

1. *Carbon Capture Inc, Bill Gross at OPTIMIZE™ 2021, Norwegian University of Science and Technology (NUST).*
2. *ExxonMobil, Don Victory at Optimize 2017 and Optimize 2021*
3. *Air Products at Optimize 2021*



Technology That Loves Complexity

About Aspen Tech.

Aspen Technology (AspenTech) is a leading software supplier for optimizing asset performance. Our products thrive in complex, industrial environments where it is critical to optimize the asset design, operation and maintenance lifecycle. AspenTech uniquely combines decades of process modeling expertise with machine learning. Our purpose-built software platform automates knowledge work and builds sustainable competitive advantage by delivering high returns over the entire asset lifecycle. As a result, companies in capital-intensive industries can maximize uptime and push the limits of performance, running their assets safer, greener, longer and faster.

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