Cover story

Digitalizing chemistry

Chemical industry embraces the future

The digital transformation of the chemical industry is underway as a growing number of companies grasp the potential of digital technologies and tools in shaping the future of chemistry. Digitalization has become fundamental to companies' strategies and is a major growth driver.

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Digitalization can make the production of chemicals more efficient and sustainable, boost innovation including the invention of novel molecules, and help solve supply-chain issues such as the serious disruption currently faced by the industry. The complexity of chemical products makes the implementation of digitalization more challenging, but chemical firms are resolutely adopting digital technologies and tools such as artificial intelligence, automation, and more recently quantum chemistry.

Specialty chemicals producer Altana (Wesel, Germany) says it has started a "comprehensive and integrated digital transformation program" including a recent €15.0-million ($15.9 million) investment in a high-throughput screening (HTS) facility at its Wesel site. Altana says the 300-square-meter facility is the largest of its type in the world and belongs to the company's largest division BYK, which produces additives and instruments.

The facility doubles BYK's capacity in application technology, Altana says. It includes 32 modules with 27 different functionalities all set to check and test BYK additives in paints, plastics, and adhesives, the company says. The HTS system performs series tests with "impressive speed and efficiency" and is able to produce and test 220 samples within 24 hours in high throughput, the company says. This is equivalent to up to 80,000 samples/year, Altana says. As a result, the time required for series testing can be cut from months to just a few days, the company says.

The time saved by the automatic series tests creates equal scope for the company's researchers, who previously had to deal with uniform series tests, to concentrate on more demanding, creative laboratory work and develop new solutions, Altana says. This provides an additional boost to the Altana's innovative prowess, it says.

The high speed of the HTS facility also allows the company to cut substantially the time-to-market phase for its customers, securing an important competitive edge for them, Altana says. "The facility operates like a giant filter. With it, we can determine with great precision which of a vast number of products tested are the two or three that will be of the greatest use and advantage to the customer," Altana says.

Existing products can also be tested to determine whether they are suitable for other areas of application, the company says. This gives rise to completely new possibilities that would be inconceivable without the digitalization of series tests, the company adds.

Altana aims to become carbon neutral by 2025 and says it is on track. "To achieve this, we have implemented a whole package of measures, such as energy efficiency, new technologies, the conversion to green electricity, and the generation of heat and power from renewable sources at our own sites," Martin Babilas, CEO of Altana, tells *CW*.

The new HTS system and other digitization initiatives will help the company achieve its sustainability targets, Babilas says. "Many people underestimate the importance of technology, its relevance for solutions to future issues," he says. "We will achieve goals such as CO_2 emissions reduction and climate protection through technologies, not only through self-limitation, and the chemical industry is at the forefront of this."

Digitalization is also helping Altana improve its customer service though a digital customer interface and an optimized customer journey overall. "A key factor is an increasingly personalized customer experience," Babilas says.

It also optimizes the utilization of the

company's plants, since production planning supported by digital tools enables optimal "on-time-in-specification" deliveries, Babilas says.

Altana is currently introducing a manufacturing execution system (MES) at its pigments business Eckart, Babilas says. MES is a computerized system designed to optimize the manufacturing process by monitoring, tracking, documenting, and controlling the entire production lifecycle.

"Overall, we have been able to establish data-science teams to fully exploit the value of data for our processes, business, and customers, [and] we constantly explore new IT digitalization technologies that help us further boost our innovation strength," Babilas says.

Solving supply-chain challenges

The usefulness of digital technologies and tools in helping solve supply-chain issues was addressed by Michael Heckmeier, executive vice president, head/display solutions business unit at Merck KGaA, during a session at CW's Specialty Strategies Forum and Innovation Awards 2022, held in May in a virtual format.

Data and digitalization for supply reliability and security form part of Merck's long-term strategy to ease the current shortage of semiconductors, caused by a variety of factors, Heckmeier said during the session.

"We have a dedicated office that looks at data from a company perspective, and we involve our customers directly through sharing data with them," Heckmeier said. "All the players need to integrate themselves and work with data-sharing models to optimize supply and demand of the whole value chain. Digitalization of the value chain will be at the end the key game to play through getting rid of redundances and bringing the various players closer together."

Machine learning algorithms can interpret data differently through multivariate analysis and identify patterns that humans and traditional quality methods cannot, Heckmeier said. "We are using this quite intensively already in semiconductor materials and, for example, in liquid crystals for displays," he said.

Merck entered into a partnership with Palantir Technologies (Denver, Colorado) in December 2021, which has been effective in helping Merck to ease the semiconductor shortages, according to Heckmeier.

The aim of the collaboration between Merck and Palantir is to deliver a secure collaborative data analytics platform for the semiconductor industry through a collaborative analytics platform called Athinia. Athinia leverages artificial intelligence (AI) and big data to solve critical challenges such as chip shortages, improve quality and supply-chain transparency, and reduce time to market, according to Merck.

Athinia brings semiconductor manufacturers and material suppliers together to share, aggregate, and analyze data to unlock efficiencies, the company says. The platform also enables industry players to understand on a deeper level the interaction between materials and processes at semiconductor fabrication plants, it says.

"The semiconductor industry is facing unprecedented disruption. This has created a critical need for a secure data-collaboration platform that can provide the transparency and data intelligence companies need to solve challenges such as chip shortages and supply-chain issues," says Kai Beckmann, board member and CEO/electronics at Merck.

Athinia enables advanced data analytics that mitigate the costly impact of quality or performance inconsistencies across the value chain, from supplier to semiconductor fabrication plants, according to Merck. It also helps fabs manage faster innovation in manufacturing processes in a single, secure platform that supports improved incoming material quality and increases supplier engagement, the company says.

BABILAS: Digital technologies support sustainability.

HECKMEIER: Data analysis can help optimize supply chains.

Digitalization was identified as one of the main factors that will affect the operation of the global chemical supply chain in a presentation by Karen Harvey, membership manager at the Chemical Business Association (CBA), the UK chemical distributors' association, during ChemSpec Europe 2022, an international exhibition for fine and specialty chemicals held recently in Frankfurt, Germany.

Chemical-industry supply chains are highly complex, and if one part is disrupted the whole chain is affected, Harvey said. Digitalization has the potential to optimize global chemical supply chains, she said.

"One of the main things about digitalization is that it is going to enable people to know where things are," Harvey tells *CW*. Innovations such as radio frequency identification technology (RFID) facilitate the wireless discovery and tracking of any object using high-frequency radio waves, she says. "Digitalization will provide much more control through being able to track where products and containers are on a global scale," Harvey says.

Supply-chain optimization in the chemicals, petrochemicals, and refining industries is also an application area of quantum computing, according to another ChemSpec 2022 presentation by Jonas Gillberg, lead/chemicals, metals, and mining industry at IBM quantum technical services. Gillberg's team is working with companies to make them "quantum ready," which means a company being "prepared and able to harness the power of quantum computing," according to Gillberg. "Quantum computing is not only a technology of the future but is also here in the present," he said during the discussion.

Quantum computers take a new approach to addressing the type of complexity found in supply chains, with the potential to discover solutions that classical supercomputers alone cannot handle, Gillberg said. Industry leaders such as ExxonMobil are becoming involved to explore how blending classical and quantum computing techniques could solve big, complex, pressing global challenges, he said.

IBM and ExxonMobil are working on finding optimal routes for a fleet of ships carrying supplies of liquefied natural gas (LNG), a critical fuel, across the oceans, according to Gillberg. This is a "mind-bendingly complex optimization problem," he said. Since 2021, more than 500 of these ships have transported LNG to destination ports around the world to power critical infrastructure, making thousands of journeys in total, Gillberg said.

Quantum chemistry

The use of quantum computing to help develop new materials is another recent trend in the chemical industry's digitalization efforts. Using quantum computing to

simulate chemical processes has become known as quantum chemistry.

According to AkzoNobel, quantum chemistry could help to overcome many of the practical boundaries associated with traditional laboratory methods such as availability of raw materials, physical equipment capacity constraints, toxicity, and environmental conditions. It could, as a result, drastically reduce the time it takes to find substitute ingredients that make products more sustainable, provide new functionalities, or replace scarce raw materials, it says.

KRUITHOF: Quantum computing will transform chemistry.

AkzoNobel recently announced a partnership with Microsoft to explore how quantum computing could help fast-track the development of high-performance and more sustainable paints and coatings.

"Quantum chemical computation is capable of simulating chemical reactions at an unprecedented level of accuracy," AkzoNobel says. Microsoft and AkzoNobel will explore how this can contribute to creating more advanced and sustainable products through collaborative experimentation and development, it adds.

"Quantum computing can be transformative for chemistry. Some chemical problems require a very high level of accuracy that's simply not attainable using traditional computers. With the availability of quantum computing, a range of chemical problems can now be tackled within an acceptable timeframe," Klaas Kruithof, AkzoNobel's chief technology officer (CTO), tells *CW*.

Quantum computing is unique in its ability to scale up very specific mathematical problems, Kruithof says. Chemistry and chemistry-related problems provide a good example, he says. "A formal treatment of chemistry-related problems requires quantum mechanics. Quantum computing is very adept at describing these quantum chemical problems and can potentially carry out these calculations several times faster than traditional computers," Kruithof says.

Pim Koeckhoven, AkzoNobel's technology director/R&D, says, "up until now, the quality of traditional computer simulations has not been up to the task. Microsoft's Azure Quantum system offers incredible opportunities for us to take our research into an entirely new digital realm and speed up the development of new novel catalysts and chemical reactions."

Simulating complex molecules and materials that have a quantum-mechanical nature can only be done accurately with quantum computing and not with traditional/classical computers, Gillberg said during his ChemSpec presentation. Quantum computers can efficiently emulate other quantum systems, such as electrons in molecules, for more predictable and accurate insights into the chemical and physical properties of complex materials. "They can help to predict the microscopic properties of materials, accelerating the discovery of new compounds, materials, processes," he said.

The applications of quantum computing in catalysis are of particular interest to chemical companies, Gillberg tells *CW*. "It is very difficult to do a computational screening of catalysts with classical computers because you cannot estimate the energy barriers accurately enough. That is why many people look to quantum computing to address this problem," he says.

The use of quantum computing to develop next-generation lithium batteries is another area of interest for chemical and automotive companies. In January, Hyundai Motors (Seoul, South Korea) and IonQ (College Park, Maryland) announced a partnership to develop new variational quantum eigensolver (VQE) algorithms to study lithium compounds and their reactions in battery chemistry.

IonQ says that quantum-powered chemistry simulation is expected to "significantly enhance the quality of next-generation lithium batteries by making improvements to the devices' charge and discharge cycles, as well as their durability, capacity, and safety."

Simulating reactions within lithium-air (Li-air) batteries using quantum computing was the subject of a recent collaboration between IBM and Mitsubishi Chemical, Gillberg said. "That was the first ever reaction simulation on a quantum computer," he said. Quantum computing can help explore effectively the reaction mechanism of li-air batteries at the atomic level, which has limited the progress of the technology, according to Gillberg. This was not possible with classical computers because the charge and discharge process in the Li-air battery are complicated and sensitive to the surrounding environment.

IBM has also worked with Daimler to publish a series of papers demonstrating progress toward using quantum computers to model material systems including Lithium-sulfur that are relevant to advancing the performance of batteries, Gillberg said.

In December 2021, quantum computing company PsiQuantum (Palo Alto, California) and QunaSys (Bunkyo, Japan), a developer of quantum algorithms and quantum chemistry calculations for materials development, launched a joint research project to assess the power of fault-tolerant quantum computing for industrial chemistry calculations. The calculations aim to accelerate the development of sustainable materials.

The companies specifically will collaborate to advance the use of quantum computing in the chemical industry, combining complementary strengths in quantum hardware, algorithm development, and materials sciences. JSR Corp. (Tokyo, Japan) has also joined the project and will evaluate quantum computing for advancements in the manufacture of photoresists, elastomers, plastics, and reagents.

JSR has also worked with IBM, using quantum computing to calculate the "excited states" of third-generation OLED emitters, according to Gillberg.

In April, DIC Corp. (Tokyo) entered into a partnership with Good Chemistry Co. (Vancouver, British Columbia, Canada) to support the realization of new materials development methods based on quantum computing and quantum chemistry technologies. Through the partnership, DIC will continue to actively promote the development of quantum-computing–driven materials development technologies that are efficient, sustainable, and clean, the company says.

DIC launched the quantum computation for chemistry (QCC) project in April 2020, with the objective of developing new technologies "for the forthcoming quantum computing era" that will advance the creation of a materials development configuration centered on chemistry simulation, the company says.

In July 2020, DIC became a founding member of the quantum innovation initiative consortium (QIIC), based at the University of Tokyo, which seeks to encourage cooperation among industry, academia, and government to accelerate quantum computing research in Japan.

DIC says it has also sought to foster opportunities for collaborative research with leading private-sector companies in the quantum computing field. ■