CAS CUSTOM SERVICES℠

DIGITAL TRANSFORMATION IN THE CHEMICAL INDUSTRY

Key steps to a sustainable future

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A division of the
American Chemical Society

Chemistry in the age of sustainability: Challenges and opportunities

Chemistry provides many of today's essentials, including textiles, pharmaceuticals, plastics, polymers, and agrochemicals. While fundamental to driving research, innovation, and economic growth, the chemistry sector also represents a major contributor to global warming.

The recurrent use of unsustainable processes within the chemical industry inevitably contributes to increasing environmental concerns. Hazardous substances, greenhouse gas emissions, or the lack of proper waste management all originate from inadequate chemical practices, which require complete reformation to meet new sustainability goals.

Recent years have seen an increased interest in digital technologies, powerful cognitive tools able to speed up innovative and sustainable solutions for the chemical industry. From better data management to improved resource use, digital transformation can empower industries by rethinking and optimizing their chemical processes, reducing their environmental impact. However, predictions for the next decade give businesses undertaking digital transformation only a 30% chance of success.[1]

Misconceptions or a poorly considered digitalization strategy can quickly transform a smart investment into a disappointment. In contrast, a deep understanding of digital technologies, their range of possibilities, and partners for strategic implementation can unravel new opportunities and help companies achieve their sustainability objectives while significantly increasing their competitiveness in the market.

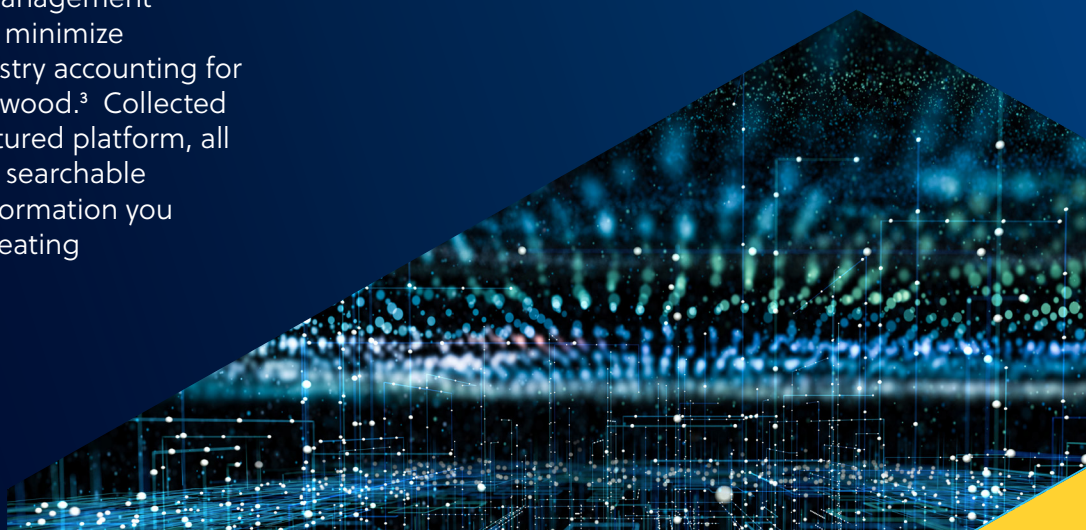
Digitalization and knowledge management: Building solid data foundations

From early-stage R&D to post-market surveillance, the chemical industry continuously generates and collects a considerable amount of data. Nevertheless, the lack of harmonization, use of different document formats, or even languages within and between organizations leads to losing valuable information and wasting precious resources. This unstructured or "dark data" counts for an estimated 55% of all stored data, significantly slowing research and innovation in the field.[2]

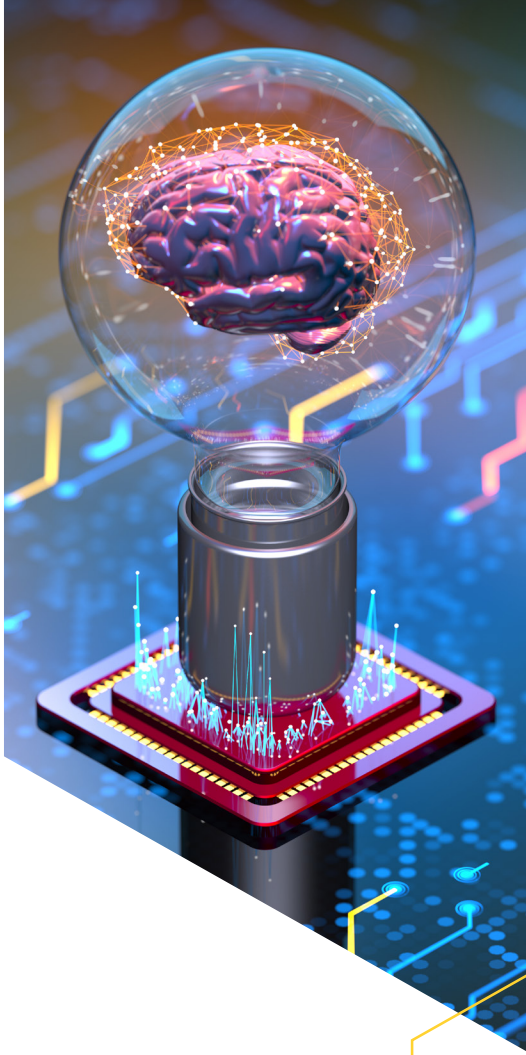
Digitalization can structure your data and laboratory while reducing your environmental footprint. Investing in a digital knowledge management system prevents data loss and can minimize deforestation, with the paper industry accounting for more than 40% of globally traded wood.[3] Collected and harmonized in a unique structured platform, all your research data becomes easily searchable in this form so you can find the information you need in record time and avoid repeating unnecessary experiments.

A decade ago, the Nature article "Scientists losing data at a rapid rate" reported that about 80% of scientific data becomes unavailable after 20 years.[4] Thankfully, the rise of digital solutions finally offers researchers opportunities to dust off their legacy scientific data and transform it into a new breeding ground for data-driven innovation.

Visit **cas.org/unravel-internal-data** to learn how CAS Custom Services℠ helped a large health-tech organization make its internal R&D data accessible.



Identifying innovation opportunities: Optimizing chemical processes with AI-enabled solutions



Today, more than 80% of chemical companies declare that sustainability has become equally as important to them as revenue growth.[5] However, despite significant practice modifications to include more sustainable options, many chemical workflows still rely on highly-polluting solvents and fossil fuels, generating hazardous waste and greenhouse gasses. Replacing each process with greener alternatives is a lengthy road requiring substantial time and financial investment. Thanks to the rise of digitalization in chemistry, cognitive tools now offer a shortcut to sustainability and innovation with an increased return on investment (ROI).

Digitalization in the chemical industry supports sustainability initiatives by highlighting new R&D opportunities. Artificial intelligence (AI)-enabled search and analytics can effectively pinpoint information relevant to your scope and objectives. By directly screening your internal database, predictive models can generate precise recommendations for better chemical formulations, sustainable manufacturing workflows, and enhanced productivity.

Adopting AI and machine learning models will ultimately bring new patent and publication opportunities tailored to your organization, increasing its general know-how, eco-friendly aspect, and competitiveness. In 2022, two-thirds of companies reported actively developing AI strategies to address their sustainability goals.[6] However, the power of AI-enabled predictions is rooted in your internal assets and can be subject to data bias.[7]

While AI-powered projects increase, organizations need solid data foundations and a robust training strategy to ensure AI accuracy.[6,8] A lack of data diversity or low quality can cause performance variations and model drift, impacting your AI predictions and leading to poor investments. Through enriched datasets and curated training sets, you can validate your predictive AI and machine learning models and identify your next breakthrough.[7]

Visit **cas.org/ai-predictions** to learn how CAS-curated training sets improved an AI model's prediction accuracy and transferability.

Visit **cas.org/predicting-new-chemistry** to learn how high-quality training data and machine learning support new chemistry.

Transitioning to sustainable chemistry: Meeting ever-changing regulatory demands

From formulation to waste management, a chemical's life cycle is subject to strict guidelines, often unharmonized between states and countries. The Food and Drug Administration (FDA), Occupational Safety and Health Administration (OSHA) European Chemicals Agency (ECHA), and Environmental Protection Agency (EPA) only represent a fraction of U.S. authorities involved in the chemical industry. In addition to the broad regulatory landscape, guidelines frequently undergo reviews and updates to align with changing scientific knowledge, technological advancements, or evolving societal expectations.

Due to their complex and evolving nature, complying with sustainability-driven regulatory demands represents a major challenge for chemical organizations. To navigate ever-changing and scattered frameworks, many chemical companies invest in dedicated regulatory affairs departments despite the financial burden. Well-implemented internal processes can significantly mitigate your costs and risks while ensuring compliance with shifting environmental policies.

Regulatory compliance typically involves extensive documentation, including comprehensive chemical records, detailed manufacturing processes, and up-to-date safety data sheets. Gathering these requirements involves browsing vast datasets from diverse departments with different methodologies. Demanding and time-consuming, this process inevitably diverts focus away from research.

Establishing a comprehensive and accurate audit trail with standardized data management systems can also help. By capturing and tracking changes made to chemical documentation through an easily searchable database, you can keep your knowledge structured, accessible, and updated as regulatory standards and environmental policies evolve.

Fast-tracking chemical innovation with CAS Custom Services: Full solution package for digitalization

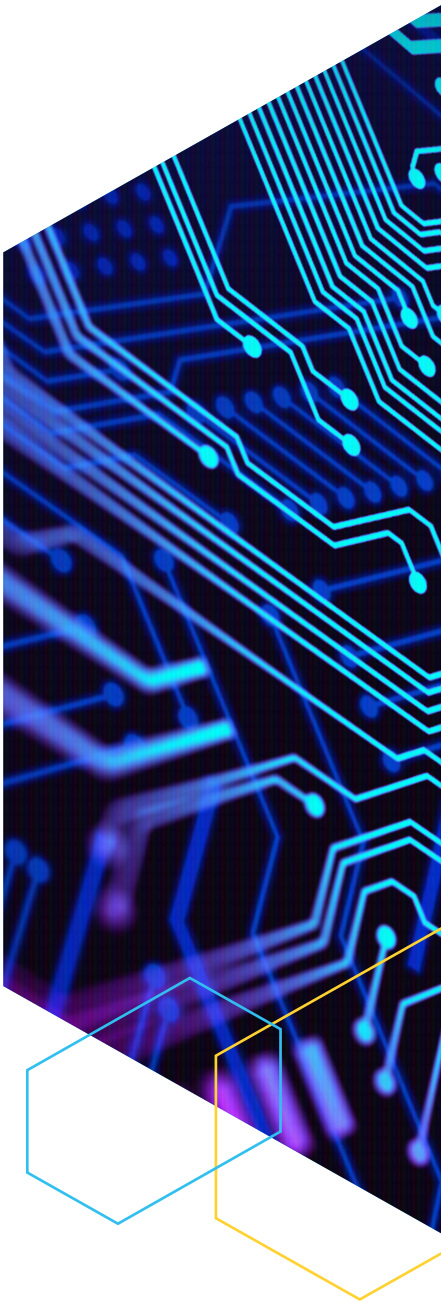
From digitizing and harmonizing a colossal amount of chemical data to training and optimizing the right AI model, digital transformation holds many growth opportunities, but they can quickly turn into delusions if done incorrectly. It is estimated that digitalization success rates in the chemical industry barely reach 15%, with 52% of chemical companies reporting skill gaps in their own workforce as a major impediment to their transformation.[9] For these reasons, numerous organizations partner with CAS Custom Services, the leader in data management, search, and retrieval.

CAS Custom Services designs tailored solutions to transform your scientific data into actionable, evidence-based insights. From data collection to connection, the cross-trained CAS team builds accessible management platforms to align with your objectives and priorities.

Digitalization possibilities are endless and provide numerous benefits:

- **Accessible, searchable assets covering all your past experiments** including digitized physical documents
- **Improved transferability and expanded application** with harmonized chemical data
- **Simplified internal and worldwide collaboration** by translating non-English documents to English
- **Quick identification of promising leads** with search algorithms and machine learning for rapid and automated data mining
- **Safer chemical formulations and sustainable workflows** with AI-enabled predictive chemical deformulation and retrosynthesis
- **Better investments and higher chances of success** with AI models trained and validated with the unique CAS Content Collection™, the world's largest chemistry data collection
- **Stress-free regulatory audits** rapidly localize the required documentation in your platform for a quick submission
- **Always up-to-date with regulatory chemical information** with CAS Chemical Compliance Index and CAS CHEMLIST

Contact one of our Solutions Consultants, and we will design a solution package tailored to your needs.



Digital transformation of the chemical industry: Cornerstone for a green future

The growing awareness of sustainability leads the chemical industry to rethink its processes, seeking eco-friendly alternatives to minimize their environmental impact and conserve resources.

Through optimized data management systems, validated AI models, and multifunctional algorithms, digital transformation is a business-changing process that provides chemical organizations significant opportunities to adopt innovative and sustainable practices in their daily operations.

By designing digital solutions tailored to your needs, CAS Custom Services can facilitate and speed up your digital transformation. Leveraging digital technologies, we can accelerate the implementation of sustainability processes in the chemical industry and considerably reduce its environmental footprints for a better tomorrow.

Visit **cas.org/contact** and start making a change today.

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