Increase productivity and reduce risk in the chemicals and materials industry

Dynamic micro- and macroeconomic factors are generating increased challenges and risks for product lifecycles, putting more pressure on decisions at chemicals and materials companies. Invaluable insights for risk mitigation and decision-making can be gained from internal and external information sources, but only if that information is properly managed and structured. Chemtiva leverages the best data science techniques and technologies to bring together critical information required for chemicals and materials companies to succeed in the new digital industry paradigm.
Digital information strategies increase efficiency, boost innovation and support effective risk mitigation.

Business risks and challenges in the chemicals and materials industry

Decision makers at chemicals and materials companies are reporting increasing challenges in the product lifecycle. These challenges include:

- Increasing energy and raw material prices
- Increasing competition due to globalization
- Need for accelerated innovation to meet customer demands
- Increasing regulatory and sustainability requirements.

Due to these increasing challenges, companies are exposed to higher risks across the whole product lifecycle: research and early development; scale-up and later development; and production and manufacturing.

Information is a key element in overcoming these challenges. Companies are looking to build risk mitigation strategies by applying cutting edge digitization techniques to fully master and information from within and external to the organization.

Digitalization presents incredible opportunities to chemicals and materials companies. It is expected to transform key aspects of the way the industry operates (1), with potential to:

- Increase efficiency and productivity
- Boost innovation
- Yield more insights from data
- Change skill and job requirements
- Change marketing and sales strategies.

“Digital will have a significant impact on many areas of the chemical industry, with the potential to change value chains, lead to higher productivity and more innovation, and create new channels to market.”

—McKinsey report on digitalization in the chemicals industry (2)
Information needs and challenges

The chemicals and materials industries have complex product development lifecycle across research, development and manufacturing. Chemists, engineers, toxicologists, and regulatory and safety professionals need to collaborate to increase productivity and make successful decisions (Figure 1). If new materials have a long lag time before bringing in revenue, this can seriously impact the company’s future. The right capabilities can dramatically speed up times to launch and meaningful revenues.

40% of revenue to come from new products developed within the last 3 years.

Customers rely on the chemicals industry to develop innovative new product.

Increased competition is driving companies to accelerate the pace of innovation.

Across product development lifecycle chemists, engineers and other professionals need to make decisions impacting product launch and commercial success. This requires information from:

- Company reports
- External websites
- Reference handbooks
- Internal databases
- Lab notebooks
- Internal portals
- Online tools

However, it is not just a question of finding the information. Across the board, professionals face challenges determining the quality of information, which may be:

- Outdated, inconsistent or untrusted
- Only available in incompatible formats
- Stored in separate or incompatible siloes
- Inconsistent with industry terminology
- Not available in searchable formats
- Behind a low-precision search interface
- Difficult to share with the right teams

Figure 1. The professionals involved in the product lifecycle must access a broad range of information to support their decisions.
Digital trends in decision making and risk mitigation

Industry giants like BASF are embracing digital business models because they see how the best technologies enable new revenue streams, increase supply shares and improve innovation through better connectivity. They also recognize how smarter supply chains and production efficiencies are supported by the optimization of all processes (3).

Applying the right data science techniques and technologies is key to success.

“The key questions for a chemical company’s management to ask are whether they’re optimally positioned and configured to take full advantage of the digital opportunity.”

—Deloitte analysis (4)

The value of digitalization

“The key findings from the analysis of [the value of digital transformation to] the chemistry and advanced materials industry the estimated cumulative economic include:

- [An] estimated cumulative economic value for the period 2016 to 2025 [ranging] from approx. $310 billion to $550 billion
- [The] potential to reduce CO2 emissions by 60–100 million tons, save 20–30 lives and avoid 2,000–3,000 injuries”

Findings of a joint World Economic Forum and Accenture study (1)

Chemtiva helps you take full advantage of digitalization opportunities

Chemtiva is a decision support solution for the chemicals and materials industries, designed to serve across the whole product lifecycle: from research and early development through scale-up to production.

It facilitates the four most important task sets for data-driven decision making and risk mitigation: aggregation, search, analytics and collaboration (Figure 2).

Figure 2. Chemtiva facilitates the most important tasks for data-driven decision making and risk mitigation.
What does Chemtiva do?

Chemtiva leverages industry best practices in data integration, domain-specific vocabularies, search technologies, text mining and data science to bring together relevant chemicals and materials information from all sources required for decision making. The capability to efficiently manage and analyze such extensive content is essential: it ensures that insights are available to all the right teams in the right formats for their work.

**Aggregation and integration:** Chemtiva brings together relevant scientific, commercial and company data for the chemicals and materials industry (Figure 3). This de-siloing and normalization ensures that every task supported by Chemtiva relies on comprehensive, trusted information.

**Search and analytics:** Chemtiva makes information discoverable by applying domain-specific taxonomies and ontologies, ensuring that search results are relevant. Visualization features help to derive insight from the trusted content. Thus, Chemtiva helps to answer a whole range of questions related to substances, products, applications and suppliers (Figure 4).

**Collaboration:** Chemtiva helps engineering, science, regulatory and EHS professionals to find and share information specific to chemicals substances, products, applications and suppliers. People supported by Chemtiva include:
- Organic, inorganic, polymer, analytical, process and formulation chemists
- EHS and regulatory professionals
- Product stewards
- Chemical, mechanical and process engineers
- Product developers

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**Figure 3.** Chemtiva operates at the intersection of external and in-house scientific and commercial data.

**Figure 4.** Examples of the applications of Chemtiva across all areas relevant for the product life cycle

- **Substances**
  - Review toxicity studies for ecotoxicity data
  - Perform regulatory and hazard comparison
  - Understand reaction pathways
  - Review technical data sheets for properties
  - Compare safety, solubility and regulatory concerns
  - Find thermodynamics data for mixtures
  - Review material compatibility for corrosiveness
  - Get latest research and experimental data
  - Optimize process equipment for new feed stock
  - Get market news and patents for competitive intelligence
  - Find commercial suppliers and pricing
  - Find alternative suppliers for scale-up

- **Products**

- **Applications**

- **Suppliers**
Integrating relevant information for product development decisions

Chemtiva integrates scientific and commercial data from external and internal sources (Table 1). The data architecture and normalization processes enable access to data for millions of chemicals and materials through a single interface. This includes secure integration of proprietary company data.

<table>
<thead>
<tr>
<th>Information type</th>
<th>Purpose</th>
</tr>
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<tbody>
<tr>
<td>Chemical regulations</td>
<td>Access thousands of global regulatory lists to assist in complying with occupational, environmental, health and safety regulations. Chemtiva contains hundreds of thousands of substances in over 5,700 lists, including non-regulatory and supplementary information.</td>
</tr>
<tr>
<td>Chemical toxicology</td>
<td>Search databases and collections that include toxicological profiles, monographs, scientific opinions, risk assessments, GHS classifications, hazard assessments, regulatory submissions, safety data sheets (SDSs), drug information, and regulatory and advisory lists.</td>
</tr>
<tr>
<td>Chemical news</td>
<td>Gain timely information essential for tracking trends and developments in the chemical and chemical engineering industries. Chemtiva is regularly updated with financial and business data from influential chemical companies, industry R&amp;D news, intelligence on government legislation changes, and analyses of economic trends.</td>
</tr>
<tr>
<td>Supplier directory</td>
<td>Find suppliers of products across a wide product range including agrochemicals, alcohols, aldehydes, ketones, organic and inorganic acids, pesticides, catalysts and polymers.</td>
</tr>
<tr>
<td>Product catalogs</td>
<td>Browse product catalogs with lab-scale pricing and supplier information for chemical building blocks and screening compounds from any supplier in any requested physical format.</td>
</tr>
<tr>
<td>Reaction pathways</td>
<td>Retrieve experimentally validated data, such as reactions (including multi-step reactions) and reaction properties (including yield, pressure, temperature, catalyst, reagents, products etc.) together with citations from chemistry journals and patents.</td>
</tr>
<tr>
<td>Chemical safety</td>
<td>See safety data sheets for products, including specialty chemicals and polymers. This information covers uses, toxicology, hazards, physical properties etc.</td>
</tr>
<tr>
<td>Technical data</td>
<td>Retrieve material properties for specialty chemicals and plastics compiled from manufacturers’ data, including physical, mechanical, thermal and application properties.</td>
</tr>
<tr>
<td>Research data</td>
<td>Find research data from many domain-specific, cross-domain and institutional data repositories including experimental data in figures, charts, tables, images etc.</td>
</tr>
<tr>
<td>Commercial shipments</td>
<td>Access global trade data from several third-party sources. This information primarily comes from customs agencies, but also includes commercial information resources of import and export details on commercial shipments worldwide.</td>
</tr>
<tr>
<td>Scientific literature</td>
<td>Search an abstract and citation database of peer-reviewed literature with titles from more than 5,000 international publishers for the most comprehensive view of the world’s research output.</td>
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Table 1. Information types that are already integrated into Chemtiva.
References


Chemtiva is a decision support solution for the chemicals and materials industries, designed to serve across the whole product lifecycle: from research and early development through scale-up to production. It leverages industry best practices to bring together relevant chemicals and materials information from all sources required for decision making. The capability to efficiently manage and analyze such extensive content ensures that insights are available to all the right teams in the right formats for their work.

For more information about Chemtiva, please contact Nina Kaun at n.kaun@elsevier.com.

Elsevier offices

ASIA AND AUSTRALIA
Tel: + 65 6349 0222

JAPAN
Tel: + 81 3 5561 5034

KOREA AND TAIWAN
Tel: +82 2 6714 3000

EUROPE, MIDDLE EAST AND AFRICA
Tel: +31 20 485 3767

NORTH AMERICA, CENTRAL AMERICA AND CANADA
Tel: +1 888 615 4500

SOUTH AMERICA
Tel: +55 21 3970 9300