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Chemicals Practice

How AI enables new possibilities in chemicals

From molecule and materials discovery to new applications and customer acquisition, AI can create opportunities across a range of promising new use cases in chemicals.

This article is a collaborative effort by Lapo Mori, Matej Macak, RS Mallya Perdur, and Yashaswi Gautam, with Ian Wells, Saumya Misra, and Zach Green, representing views from McKinsey's Chemicals Practice.
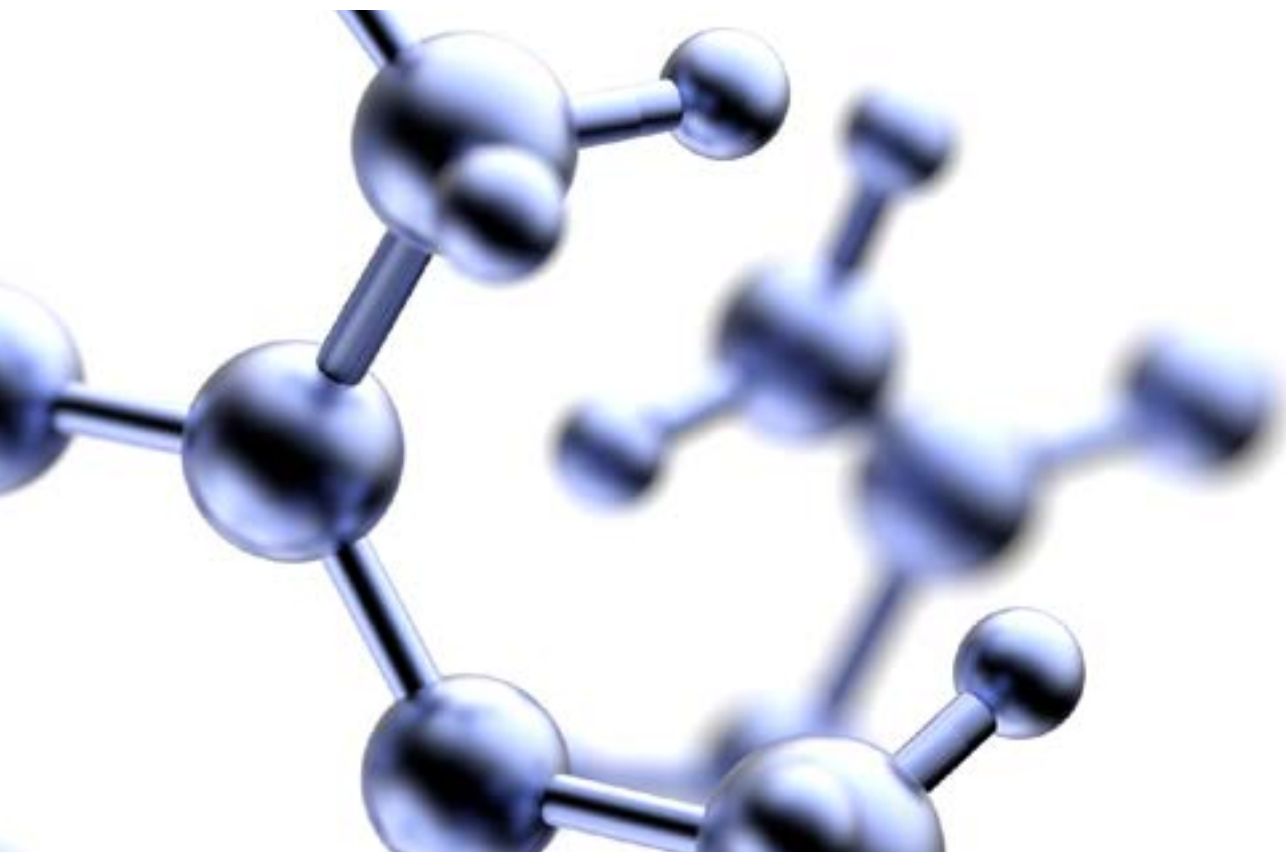
It has been nearly two years since the launch of ChatGPT and other generative AI (gen AI) tools that revolutionized the way AI is perceived and consumed by industries, businesses, and other users. In that time, McKinsey experts estimate the capabilities unlocked by gen AI have helped accelerate levels of human performance by a decade, on average.[1]

No industry remains untouched by the impact of gen AI, but adoption levels vary significantly. The chemical industry, in particular, remains a cautious adopter. A recent McKinsey Global Institute (MGI) survey estimates that energy and materials, which includes chemicals, has the lowest exposure to gen AI tools at 14 percent, compared with the cross-industry average of 23 percent.[2] Meanwhile, chemical companies have significant untapped potential to leapfrog competitors using the recent advancements brought about by generative technologies.

This potential stems from the industry's reliance on scientific data for innovation, the availability of (often fragmented) customer data, and the industry's nuanced and complicated manufacturing processes.[3] Simply stated, gen AI adds intelligence and completeness to these data, which can then be used to inform decision making, speed up processes, and improve overall efficiency. Altogether, our estimates show the application of gen AI across commercial, R&D, operations, and support functions in energy and materials can create anywhere from $80 billion to $140 billion in value.

Harnessing this new technology won't be easy. Many use cases cannot be realized unless some degree of digitalization, technical capability, and scientific expertise is already in place. This article provides an overview of today's most relevant opportunity areas and offers a pathway for chemical industry players to start taking concrete actions.

Chemicals and AI: An overview

The chemical industry plays a critical role in the global economy, providing essential materials for most other industries. Today, chemical companies face market forces that require new ways of thinking, including the search for newer materials to support the future innovation needs of the energy transition.[4] Other forces include reinvigoration of growth with both new and existing customers, efficiencies in manufacturing and supply chain to fund growth and innovation, and significant talent and capability attrition as the workforce turns over.

"Gen AI" refers to applications that can process varied sets of unstructured data (such as lab notes, technical specification sheets, scientific literature, and sales presentations) as well as structured data (such as customer relationship management and transactional data) to aid synthesis, suggestions, and new content generation. In this way, gen AI generates new ideas by identifying patterns in data sets, particularly when it comes to complex tasks such as finding new applications, customer acquisition, and molecule or materials discovery. By contrast, more traditional, analytical AI typically solves specific tasks by analyzing data and making predictions based on structured data sets and predefined rules.

AI and gen AI are not competing technologies; rather, they can complement each other. The combination of the two technologies, referred to here as "gen AI," has the potential to transform nearly all aspects of the chemical industry, revamping the ways companies operate and potentially unlocking billions of dollars in value. Although core pricing and forecasting models will likely continue to be based on traditional AI, generative technology allows organizations to prepare data faster, tap into internal and external sources, and support conversational abilities that can lead to pricing or forecasting insights.

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[1] *The economic potential of generative AI: The next productivity frontier*, McKinsey, June 14, 2023.
[2] "The state of AI in 2023: Generative AI's breakout year," McKinsey, August 1, 2023.
[3] "Beyond the hype: New opportunities for gen AI in energy and materials," McKinsey, February 5, 2024.
[4] For more on materials and the energy transition, see *The net-zero materials transition: Implications for global supply chains*, McKinsey, July 5, 2023.

Chemical companies have significant untapped potential to leapfrog competitors using the recent advancements brought about by generative technologies.

Companies will likely need to have a combination of digitalization, technical capabilities, and scientific expertise before they can harness the potential of AI, and not every use case will apply across the board. The potential risks of AI must also be accounted for, including the accuracy of responses, security from cyberattacks, protection of competitively sensitive data, biased outputs, and the risk of intellectual property infringement.[5]

The AI opportunity in chemicals

Innovation in the chemical industry has been slow. As a point of comparison, Amazon spent $73 billion on technology and infrastructure (a major component of which was R&D) in 2022,[6] while the entire US chemical industry spent $13 billion.[7] Some of this slowness is structural, arising from the industry's asset-heavy nature, longer innovation cycles compared with software or consumer goods, enhanced regulatory considerations, and less-distributed customer base (primarily due to the B2B nature of offerings). However, the industry has also been a late adopter of new technologies and has subsequently been slow to deploy them to derive business value.

In the chemical industry, gen AI represents a substantial leap forward, making the generation of insights and creative processes, such as new molecular and marketing designs, more accessible and customizable. This democratization of technology can help companies, especially those with below-average performance, significantly enhance their operations.

Moreover, gen AI is reshaping competitive landscapes by enabling new ways to generate hypotheses using diverse data sources, augment individual creativity with systematic support, and embed tacit knowledge into institutional advantages. This evolution reduces entry barriers for new players, which can now use customer data more effectively and offer their products without traditional constraints. In addition, customers could gain the ability to easily compare and select suppliers, thanks to increased transparency. These shifts suggest that future competitive advantages in chemicals will rely heavily on the strategic use of AI.

Although gen AI was initially seen as a productivity lever, over the past year some organizations have uncovered its growth potential as well, particularly in new-customer identification and account management. The following 11 use cases cover three chemical domains that McKinsey experts regard as having the greatest potential for near-term impact (Exhibit 1).

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[5] For more on these risks, see "Beyond the hype," February 5, 2024.
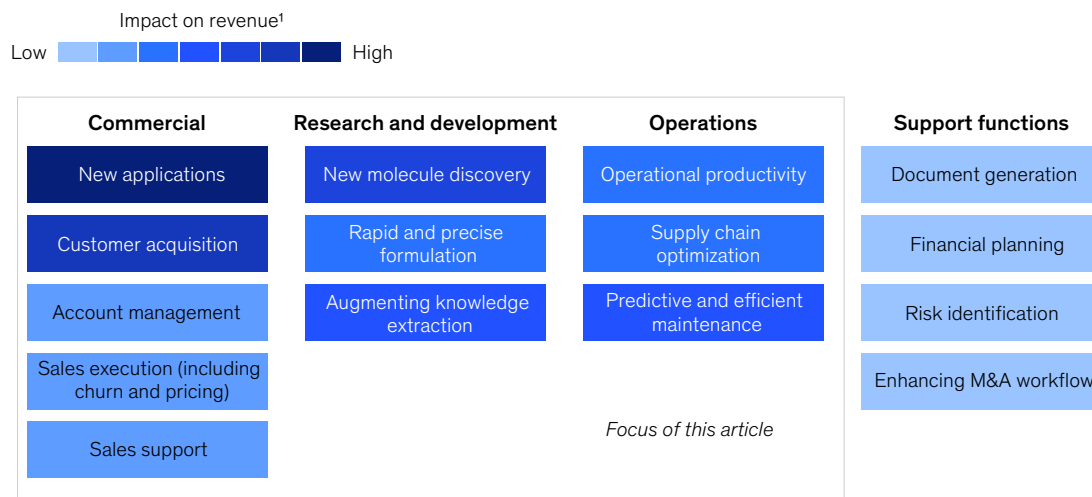[6] *Annual report*, Amazon, 2023.
[7] "Chemical industry research and development spending in the United States from 2014 to 2022," Statista, May 22, 2024.

Exhibit 1

Generative AI can help create value across all business functions in chemicals.

Impact of generative AI use cases on functions across businesses

Impact on revenue[1]

Low ▢▢▢▢▢▢ High

Commercial	Research and development	Operations	Support functions
New applications	New molecule discovery	Operational productivity	Document generation
Customer acquisition	Rapid and precise formulation	Supply chain optimization	Financial planning
Account management	Augmenting knowledge extraction	Predictive and efficient maintenance	Risk identification
Sales execution (including churn and pricing)			Enhancing M&A workflow
Sales support		*Focus of this article*	

[1]Impact is based on a percentage of revenue for each step in the value chain, using historical data from the chemical industry.

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Commercial

The commercial cycle in chemicals ranges from customer identification to the development of repeat purchases (Exhibit 2). Gen AI has various use cases across the chemical commercial cycle, including new applications, new-customer acquisition, strategic account management, sales execution (including pricing and churn management), and sales support.

New applications
Potential impact: Reduce time required to find new applications from months to days

Gen AI can be a powerful tool for discovering new applications for existing chemicals. By analyzing vast amounts of external and unstructured data from various sources, including patents, publications, and industry news, gen AI can identify potential new markets and applications not previously considered. It can also significantly reduce the time spent in application identification and developing business cases. Moreover, gen AI

can prioritize these opportunities based on potential market size and growth, helping businesses focus their R&D and marketing efforts on the areas with the most promise. Ideally, this process will not only speed up the innovation cycle but also open new revenue streams by extending the utility of existing products.
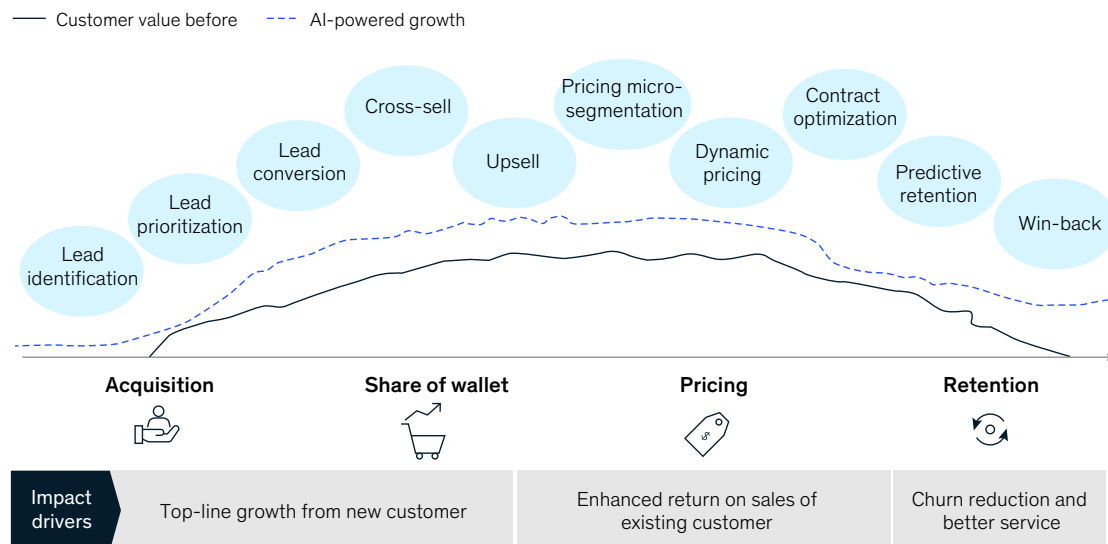
Customer acquisition
Potential impact: Increase the rate of new customer growth and sustain revenue uplift of 10 to 20 percent

It can be challenging to find new customers that are likely to be users of a particular product. Many companies take a structured approach to identifying new customers only for the largest customers, taking a reactive approach to the rest. But gen AI is reshaping how organizations discover and engage with new customer segments. By deeply analyzing vast data sources such as web content, scientific literature, company reports, and market updates, gen AI can reveal new opportunities for growth. Doing so can streamline

Exhibit 2

Generative AI can enhance performance across the customer life cycle in chemicals.

Customer lifetime value

Customer value before ⸺⸺ AI-powered growth - - -

Lead identification · Lead prioritization · Lead conversion · Cross-sell · Upsell · Pricing micro-segmentation · Dynamic pricing · Contract optimization · Predictive retention · Win-back

	Acquisition	Share of wallet	Pricing	Retention
Impact drivers	Top-line growth from new customer		Enhanced return on sales of existing customer	Churn reduction and better service

the lead generation process, singling out the most promising prospects for engagement and conversion. Gen AI can also integrate and learn from historical transactional data, refining customer profiles for precision targeting. This can result in a more strategic deployment of marketing and sales resources, optimizing customer acquisition and fostering sustainable business growth. Precision targeting via gen AI also offers the ability to empower inside sales and engage moderate- to low-volume customers appropriately through the conversion funnel and, if needed, handing them back to the sales representative when they are on the cusp of making a purchase decision.

Strategic account management
Potential impact: 20 to 30 percent more incremental opportunities in the development pipeline

Many organizations struggle to turn key account management practices into real growth drivers for the business. For instance, they often do key account

management in a checklist-like manner by looking into historic trends to identify future opportunities or by reactively addressing customer needs.

Gen AI tools can help users understand the broader business context and strategy of a customer by tapping into public reports, which can then be translated into the likely implications for end markets. These insights can then be converted into opportunities for specific products. In simpler applications, gen AI can look into customer segment information internally as well as the opportunities being pursued by commercial teams globally to suggest new opportunities a particular account manager may not be considering.

For example, a large chemical company recently looked into the opportunities that its product's unique properties could have in a particular end-market application. Using gen AI, this company was able to understand not only the structure of the application market but also the concrete

opportunities it could pursue with its customers. As a result, an additional, previously unexplored opportunity was created in the pipeline for commercial teams.

Sales execution (including pricing and churn management)

Potential impact: Optimize pricing in real time to secure 2 to 5 percent return on sales and reduce revenue churn by 10 to 20 percent, compared with historic rates of attrition

Advanced pricing requires access to large amounts of data—for example, payment terms, customer visit reports, customer expansion plans, and buying patterns. However, these data are often fragmented and of varying quality, making them difficult to analyze and use effectively. To gain an edge, companies can use gen AI to analyze more than a dozen pricing inputs (including market data, competitor prices, buying patterns over the past ten years, and consumer behavior) and set dynamic pricing strategies. Advanced pricing is enabled through the following three levers:

— *Comprehensive customer analytics.* Analyzing vast amounts of data and identifying patterns and trends in consumer behavior allow companies to gain insights into customer preferences, buying behavior, and price sensitivity.

— *Real-time pricing adjustments.* Dynamic pricing allows companies to respond quickly to market fluctuations and optimize their pricing strategies accordingly. For example, if there is a sudden surge for a certain polyethylene grade, AI can automatically raise prices to maximize profits.

— *Unlock interdependencies.* Analyzing the impact of slight price adjustments across an entire category can provide a more comprehensive view—for example, showing how a change in the pricing of one product can affect sales of other products in the portfolio.

Gen AI can also be used to monitor risk for churn and customer retention by analyzing a variety of data sources, such as financial reports, market analytics, and transactional data. It can spot market

and customer trends, turning them into early indicators of customer disengagement and enabling businesses to proactively address churn risk. As an example, traditional AI-based predictive churn models can be enriched with external data, such as social media commentary or earnings estimates. By evaluating these insights, companies can make better decisions to prevent customer loss. Finally, gen AI can speed up the response time to these risks, allowing for quick and targeted customer retention strategies, including personalized offers and promotions addressing identified churn drivers.

Sales support

Potential impact: Up to 20 percent of seller capacity redeployed for growth

Gen AI can propel sales teams forward by consolidating complex customer data into a single, actionable view, enabling richer customer understanding and better execution focus. It can also help standardize salesforce capabilities across regions—for instance, the salesforce close to headquarters can more easily bring the remote salesforce up to speed on current and new products. This unified system offers a comprehensive understanding of customer needs, driving personalized engagement and tailored sales approaches. In addition, real-time assistance from gen AI chatbots can provide immediate access to crucial information—from competitor analysis to multilingual support—helping sellers adapt and respond in the moment. The result is a streamlined sales process that not only frees up more time to sell but also enhances the overall selling experience.

As an example, a North American chemical company leverages gen AI to address challenges in executing commercial excellence levers. Company leaders identified a lack of understanding of expected commercial actions among sales team members, which caused significant value leakage. Using gen AI, the company is integrating a conversation interface into its customer relationship management system, which offers targeted commercial-action triggers for sales reps and enables reps to query and understand the rationale for commercial actions. Although many high performers in sales organizations are skilled at pursuing some sales augmentation practices in their own intuitive ways, gen AI allows organizations to significantly lift low performers.

Research and development

Today, R&D processes in chemicals take a long time. The discovery of new molecules or materials can take several years and require tens of millions of dollars in research funding from conception to at-scale deployment. However, gen AI tools promise to augment the innovation cycle through faster discovery, net new molecule or material identification, and rapid and precise formulations, as well as efficient leveraging of internal and external R&D knowledge to augment the metabolic rate of innovation.

Foundation models that sit at the core of R&D acceleration are more data efficient and can be powerfully deployed in closed-loop research systems (CLRS), optimizing research innovation. As a result, the number of R&D iterations and the requisite data can be drastically reduced compared with traditional AI (in some cases by 90 to 99 percent).

With all of this in mind, emerging generative AI approaches have demonstrated value for three areas of focus: new molecule or material discovery, rapid and precise formulation, and augmented knowledge extraction.

New molecule or material discovery

Potential impact: Two- to threefold acceleration in materials or molecule discovery with net new patentable chemistries discovered and optimized for end-state product properties

Some discovery challenges across chemicals require significant amounts of time. For instance, new formulations can help optimize costs or performance, new molecules can be more sustainable (such as those free of per- and polyfluoroalkyl substances, or PFAs), and the relevant properties of materials can be improved (such as thermal and hydrothermal stability for catalysts in petrochemicals).

For example, a chemical company in North America recently looked into the possibility of formulating a new coating to address challenges it faced in one of its end-market application. Using gen AI, the company mined the universe of materials using external data as well as its own proprietary R&D data and ultimately identified the molecules that could offer the desired functionality. This allowed the company to move from a slow and expensive user-customization cycle to a rapid customization cycle at a fraction of the cost.

Gen AI models can also dive into huge amounts of public data (such as patents, publications, and grants) and suggest chemistries or formulations to be tested in the lab or end-state processes, requiring significantly less data than traditional AI for training or fine-tuning. The results from lab experiments or scale-up testing are then fed back into the models to further improve the properties, resulting in a discovery flywheel. Google DeepMind, for example, has already predicted structures for 2.2 million new materials, of which more than 700 have been created in the lab and are now being tested.[8]

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[8] Ekin Dogus Cubuk and Amil Merchant, "Millions of new materials discovered with deep learning," Google DeepMind, November 29, 2023.

Gen AI tools promise to augment the innovation cycle through faster discovery, net new molecule or material identification, and rapid and precise formulations. . . .

Rapid and precise formulation

Potential impact: More than 30 percent acceleration in achieving the desired formulation and approximately 5 percent savings on cost

Achieving the specifications required by customers or target functionality profiles requires multiple iterations as well as the expertise of the individual formulator. In some cases, formulations are overspecified, which can add to the cost. With this in mind, there are typically two levers of value creation: 1) optimizing formulation specifications to be "good enough" for a given application (minimizing overspecification), and 2) recommending the lowest-cost formulation (based on the identity and ratio of various raw materials) to meet the required specifications.

In addition to optimizing raw-material costs, there are opportunities to optimize production processes (such as temperature and processing time) and therefore reduce energy costs. Achieving this, however, entails foundation models and large language models

(LLMs) to discover relevant chemistries from existing databases, patents, literature, and other sources. Doing so can help aid the discovery of chemicals used to optimize properties or as substitutes in the formulation design to improve cost.
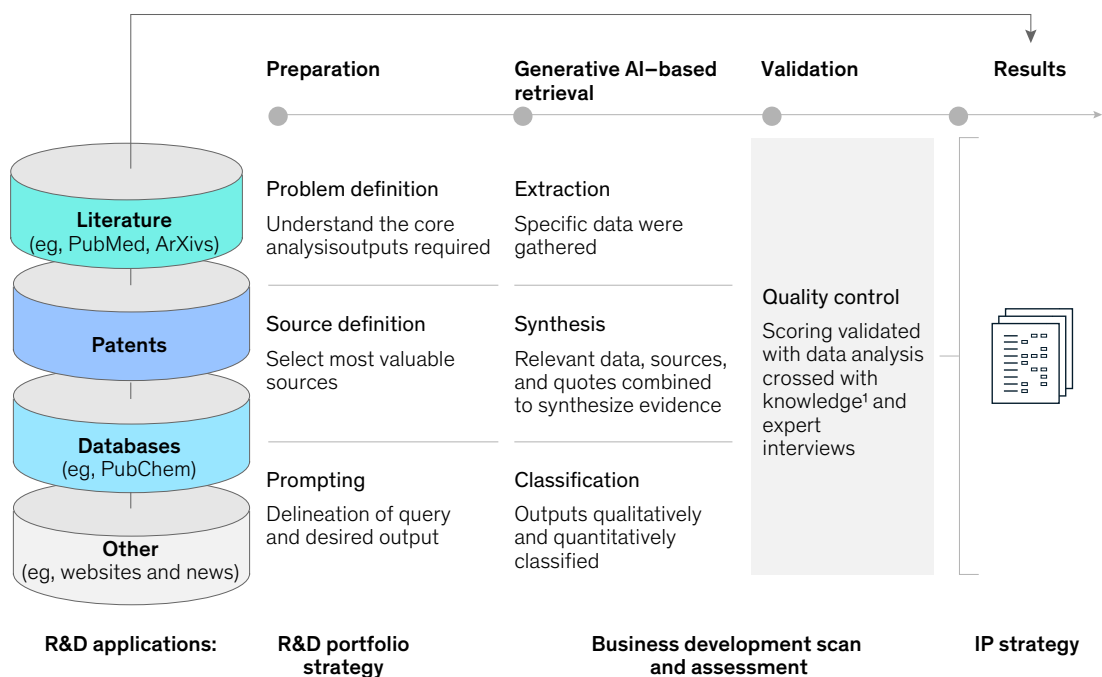
Augmented knowledge extraction

Potential impact: More than 30 percent increase in initial manual assessments of literature

In chemicals, scientists often spend considerable time extracting and summarizing information from diverse sources such as patents and scientific literature to better understand molecular or material properties and reaction mechanisms. This process is labor-intensive and prone to incomplete or inaccurate information due to the vast amount and diversity of data involved. By contrast, gen AI can greatly enhance the extraction of scientific knowledge through efficient data management (Exhibit 3). In addition, integrated proprietary data can be searched and queried in a simple text- and dialogue-based interface.

Exhibit 3

Generative AI can rapidly synthesize and score evidence across a broad scope of scientific data sources.

	Preparation	Generative AI–based retrieval	Validation	Results
Literature (eg, PubMed, ArXivs)	**Problem definition** Understand the core analysis outputs required	**Extraction** Specific data were gathered	**Quality control** Scoring validated with data analysis crossed with knowledge[1] and expert interviews	
Patents	**Source definition** Select most valuable sources	**Synthesis** Relevant data, sources, and quotes combined to synthesize evidence		
Databases (eg, PubChem)				
Other (eg, websites and news)	**Prompting** Delineation of query and desired output	**Classification** Outputs qualitatively and quantitatively classified		

R&D applications:	R&D portfolio strategy	Business development scan and assessment	IP strategy

[1]Based on availability, validity, and strength of scientific knowledge identified.

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As an example, a European chemical player deployed gen AI to automatically collect data from connected lab instruments and allow scientists to record notes from anywhere in the lab. In turn, researchers gained access to the scientific protocols, and any aberrations were immediately highlighted.

Gen AI in R&D can also facilitate communication and collaboration among scientists, helping them share best practices and lessons learned. This essentially provides real-time feedback and suggestions, helping scientists adapt to new technology more quickly and effectively. It also allows scientists to better track progress and measure the impact of the new technology, providing valuable insights for continuous improvement.

Operations

Chemical manufacturing processes produce vast amounts of structured and unstructured data that have until now been too unwieldy for traditional analytics. With AI-powered models, however, these data can be easily processed to improve predictive and efficient maintenance, operational productivity and throughput, and supply chain optimization.

Predictive and efficient maintenance
Potential impact: 30 to 40 percent increase in maintenance labor productivity

One crucial aspect of maintenance in chemicals is understanding equipment failure modes and developing mitigation strategies that balance cost and risk. Some companies are leveraging gen AI to instantaneously create or enhance failure modes and effects analysis (FMEA) by combining their internal maintenance histories with publicly available data (Exhibit 4).

In addition, recent advances in AI image recognition and processing can help operators identify

Exhibit 4

Generative AI can rapidly process reliability data to identify root causes, flag bad actors, and evolve preventive-maintenance programs.

1. Generate FMEA
Create a failure modes and effects analysis (FMEA) from an asset description

2. Analyze work orders
Evaluate work orders (with equipment description and maintenance activities) and optionally FMEA to derive failure mode labels

Reliability copilot process

3. Accelerate reliability analysis
Combine FMEA, work order failure modes, and maintenance history to identify bad actors and assess preventive-maintenance (PM) effectiveness

4. Optimize maintenance strategy
Review bad actors list and PM effectiveness and evolve maintenance strategy with copilot suggestions
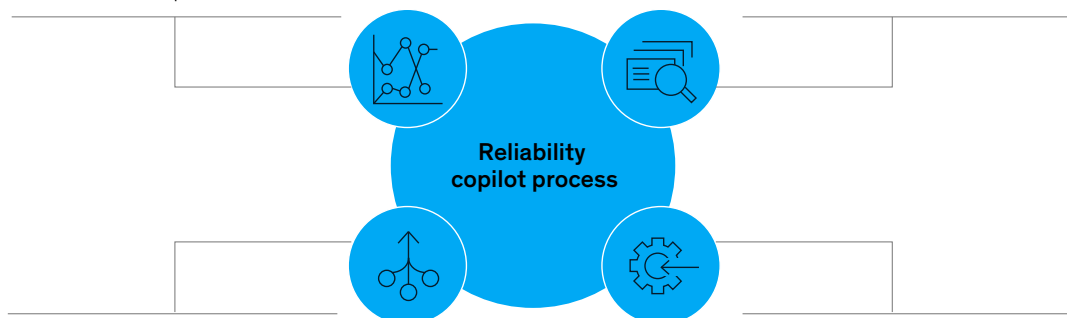
Source: QuantumBlack, AI by McKinsey

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anomalies and predict failures in the field. In turn, this enables preventive maintenance and improves equipment uptime. AI can also generate maintenance plans by ingesting OEM manuals, preexisting job plans, maintenance assessments, and parts catalogs. As an example, one chemical company created a "maintenance virtual expert" for processing equipment maintenance, which answers the questions of technicians, diagnoses issues, and creates procedures and work instructions that link to the work order system, massively improving technician productivity and manufacturing equipment uptime.

Operational productivity and throughput
Potential impact: More than 10 percent increase in yield and throughput

Real-time process optimizers have been deployed to process sensor data in near-real time and help control room operators make decisions to maximize yield, energy, and throughput. By layering gen AI, these optimizers can quickly and accurately answer technician queries and explain model recommendations, increasing operator confidence and adoption. Another useful gen AI application in operations is control room copilots, which can tap into vast technical documentation and provide live troubleshooting advice. AI can also suggest changes to the production schedule to minimize downtime and maximize throughput, as well as identify the optimal temperature, pressure, and flow rates for particular chemical processes.

Supply chain optimization
Potential impact: Reduce lost sales related to customer service by more than 65 percent and save on administrative costs by more than 50 percent

Rapid insight generation is one example of how AI can converse with supply chain employees, synthesize unstructured real-time data to identify root causes and trends, detect potential disruptions, and suggest remediations for exceptions. AI tools can also automate the evaluation of various supply chain scenarios, simulating potential network scenarios to optimize inventory levels and cost.

Next-generation cross-functional orchestration is another way in which AI acts as a smart intermediary, connecting planning systems and optimization libraries to automatically answer questions related to inventory recovery and processes, and facilitating coordination with external stakeholders. Virtual assistants can aid in creating internal documents, such as process descriptions and dictionaries, and preparing documents for sales and operations planning. In addition, AI can enhance customer service by providing instant responses to questions related to order delivery, inventory recovery, new products, and more. However, this requires data policy decisions for customer rollout.

Harnessing the potential: How to capture value from AI in chemicals

Many chemical companies are still in the early stages of their AI journeys and therefore need to act quickly to capture maximum value. The technology is there—but the solution is not "just the tech." Companies will need to employ the tech while capturing value and managing change. This means companies will need to plan with key players in the business to ensure that decisions are powered by AI insights and that custom solutions are built with AI at the core, all while constantly refining these tools based on real-world feedback.

First and foremost, leaders must understand that AI cannot be a peripheral initiative; it should be a top priority. Given the conservative nature of many large organizations, C-suite executives must make a genuine commitment. Second, although organizations must move quickly to seize the competitive edge, attempting too much too soon can be problematic. And third, organizations must go beyond the pilot level and create a clear road map to realize the full potential of AI.

Organizations can start the AI journey by taking a two-pronged approach: 1) starting with targeted opportunities that can quickly deliver impact and build excitement within the business, and 2) exploring use cases that will fundamentally alter the business. By adopting this approach, organizations can strategically balance quick wins to maintain momentum and support for transformative changes that prepare the business for future challenges and opportunities.

That said, these opportunities often need insights derived from third-party data or internal "messy" data, require a deeper dive into IT and digital infrastructure, necessitate meaningful downstream process redesign to be embedded into the workflow, and demand significant change management to capture the full value of the initiative.

As organizations develop their use cases, they need to comprehensively transform across the following dimensions to unlock the complete potential of AI:

— *Develop a strategic road map.* Align the gen AI strategy with the broader technology goals of the organization. Approach the transformation in a manner that captures value and secures a competitive edge.

— *Manage talent.* Address the AI skill gap by effectively managing and developing talent. This ensures the organization remains ahead in gen AI capabilities.

— *Optimize operational model.* Organize teams and structures within the organization to effectively deliver on the generative AI strategy.

— *Build technology infrastructure.* Establish a scalable technology stack and infrastructure that can support multiple generative AI use cases and solutions.

— *Establish a data foundation.* Create a robust data foundation that can support the scaling of gen AI across the organization. The barrier for data quality and quantity is fairly low when it comes to creating value from AI, which means the value created from AI can be a driving force for better capturing data.

— *Implement change management.* Design a scaling plan that allows for easy reusability and scalability of AI capabilities. Provide effective training to support skill building and manage cultural change within the organization. Also, address risks and promote the responsible use of gen AI.

The companies that most benefit from AI will likely be incumbents with decades of commercial, operational, or R&D data or newcomers seeking to leverage AI and external data to more quickly close the gap with incumbents.

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From the automotive industry to pharmaceuticals to manufacturing to agriculture, the chemical industry plays a critical role in any number of everyday products and processes. In turn, the application and acceleration of AI will have far-reaching effects. The timing is right for digitalization, technical capabilities, and scientific expertise to align, enabling companies to apply AI across all functions. Those that move quickly could see outsize value in both the near and long term, and those that hesitate risk falling behind.

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