Agentic AI in Chemical Engineering 5.0: current landscape and future outlook

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ABSTRACT
The convergence of Chemical Engineering 5.0 and Agentic Artificial Intelligence (AI) marks a paradigm shift in the chemical industry. Unlike traditional AI, intelligent agents do not just analyze data; they reason, plan, execute complex tasks in closed-loop systems. Today, this technology optimizes operational efficiency in chemical plants through advanced predictive maintenance and autonomous real-time tuning of process variables, drastically reducing energy consumption and carbon footprints. In the near future, Agentic AI will be the cornerstone of Self-Driving Labs, where multi-agent systems will independently design new catalysis and materials by integrating molecular simulation and robotic experimentation without constant human intervention. This evolution toward a human-centric industry' will allow engineers to shift into strategic and ethical oversight roles, while agents manage supply chain resilience and industrial symbiosis. Therefore, the primary goal of this work is to demonstrate how Agentic AI is not merely a computational tool, but an essential autonomous collaborator for achieving sustainability and mass customization that defines the era of Chemical Engineering 5.0.

Keywords: Chemical Engineering 5.0, Agentic Artificial Intelligence, Sustainability, Self-Driving Labs.

1 INTRODUCTION

Chemical Engineering 5.0 represents the discipline's most ambitious evolutionary leap. It is the natural evolution of digitalization toward a model where technology and human ingenuity collaborate symbiotically. While Industry 4.0 focused on digitalization and connectivity (the "Internet of Things"), Industry 5.0 centers on deep collaboration between humans and Artificial Intelligence (AI), radical sustainability, and mass customization (Boskabadi *et al*., 2025).

In 2026, it is no longer just about producing 'more for less,' but about producing intelligently, ethically, and in harmony with planetary boundaries. To achieve this, Artificial Intelligence has moved beyond being a 'support' tool to become the core engine of Chemical Engineering 5.0. Integration is no longer just digital, but physical (robotics) and biological (biotechnology) as well. Today, AI is applied everywhere, from the laboratory to the industrial plant (Elghany & Elessawi, 2026).

Chemical Engineering 5.0 is the evolution of the discipline that integrates the advanced digital technologies of Industry 4.0 (AI, IoT, Big Data) with a deeply human-centric, resilient, and sustainable focus. While the previous stage (4.0) was obsessed with efficiency and automation— 'machines talking to machines' (Abdulrazzq *et al*., 2024; Cruz-Olivares *et al*., 2026)— Chemical Engineering 5.0 seeks to ensure that technology serves to enhance human talent and regenerate the environment.

The fundamental pillars of Chemical Engineering 5.0 are as follows (Cimino *et al*., 2025; Díaz-Martínez *et al*., 2026):

1.1 THE 5.0 ENGINEERING FRAMEWORK

To understand this new era, we must examine how three key concepts intertwine:

- *Radical Sustainability:* It is no longer enough to simply 'pollute less.' Processes are now designed for negative emissions (CO_2 capture) and a circular economy where waste is non-existent by design.
- *Resilience:* The capacity of chemical plants to adapt to crises (pandemics, wars, climates change). This is achieved through modular plants that can be reconfigured in days rather than years.
- *Human-Centric Focus (Bio-Synergy):* AI does not replace engineers: it liberates them from repetitive and hazardous tasks so they can focus on innovation, ethics, and complex problem-solving.

1.2 DEFINING TECHNOLOGIES OF ENGINEERING 5.0

What separates 4.0 engineer from 5.0 engineer is the use of the following tools:

- *Agentic AI:* Systems that do not just predict but make autonomous decisions within the plant, operating within ethical and safety boundaries defined by humans.
- *Cobotics (Collaborative Robotics):* Robots that work shoulder-to-shoulder with engineers in laboratories or plants, capable of learning from human movements.
- *Cognitive Digital Twins:* Virtual replicas of the plant that 'think' and simulate decarbonization scenarios in real time.
- *Programable Biomanufacturing:* The use of computer-designed cells and enzymes to replace heavy petrochemical whit room-temperature fermentation.

Table 1 and Figure 1 provide a brief comparison between Chemical Engineering 4.0 and Chemical Engineering 5.0.

Table 1

Chemical Engineering 4.0 vs. Chemical Engineering 5.0

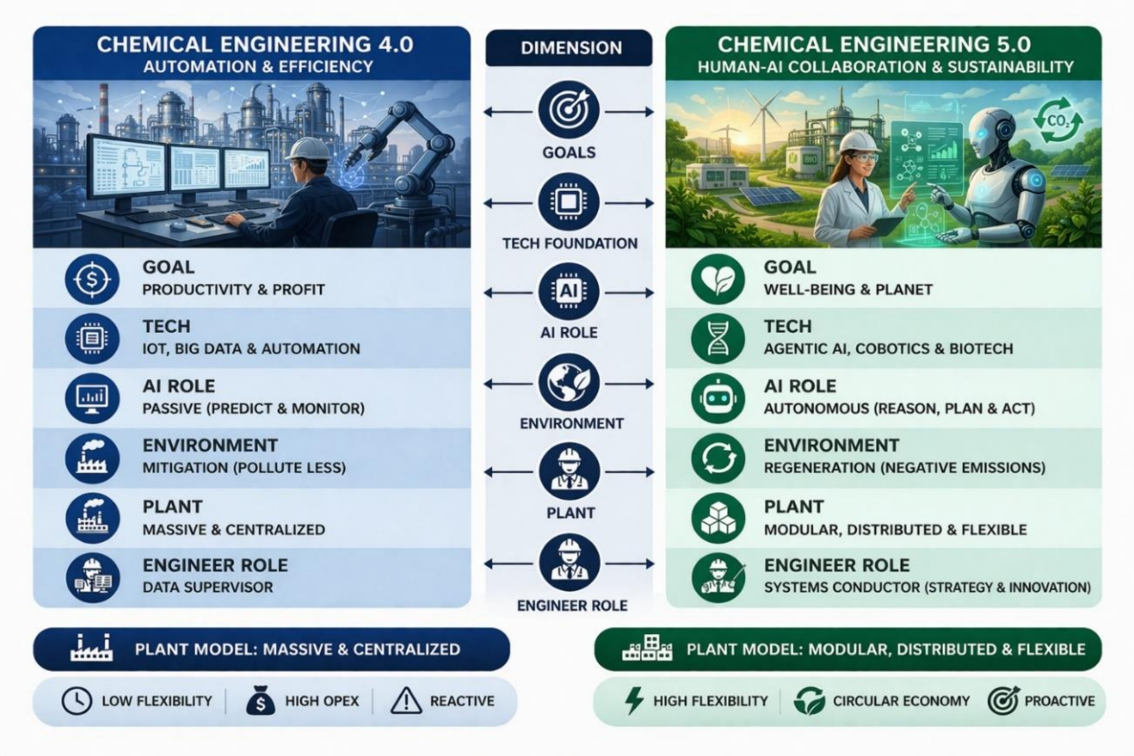
Feature	Chemical Engineering 4.0	Chemical Engineering 5.0
Primary Goal	Productivity and Profit.	Human Well-being and the Planet.
Core Technology	Automation and Internet of Things (IoT).	Agentic AI and Biotechnology.
Role of the Engineer	Screen and data supervisor.	Architect of sustainable systems.
Plant Model	Massive and centralized.	Modular, distributed, and flexible.

Environmental Impact	Mitigation (reducing damage).	Regeneration (restoring the environment).

For Mexico, Chemical Engineering 5.0 represents a golden opportunity within the framework of nearshoring. By adopting 5.0 technologies, Mexican plants can address the climate crisis and the need for industrial sovereignty, creating green intellectual property and processes thar comply whit global 'Net-Zero' laws. Consequently, this paper provides a brief description of the importance and relevance of integrating Agentic Artificial Intelligence with Chemical Engineering.

Figure 1

Comparison of Chemical Engineering in industry 4.0 and 5.0



Source: From the authors by means of artificial intelligence

2 METHODOLOGY

2.1 AGENTIC ARTIFICIAL INTELLIGENCE (AGENTIC AI)

Agentic Artificial Intelligence is an emerging area within the field of AI, characterized by the development of autonomous systems capable of independently pursuing complex goals with minimal human intervention. These systems are designed not only to set and refine their own objectives but also to formulate and execute multi-step strategies, leveraging various tools and resources to optimize task completion (Holldack *et al*., 2026). Unlike traditional AI methods that operate on structured instructions and strict supervision, these systems possess the capacity for dynamic adaptation, allowing them to adjust their action in response to changing environmental conditions or unforeseen challenges without human intervention to achieve them. This adaptability enhances their operational autonomy and enables more efficient problem-solving across diverse contexts. Furthermore, Agentic AI systems are designed to ensure the accuracy, clarity, and relevance of their output, thereby facilitating the achievement of user-defined goals (Allmendinger *et al*., 2026).

Its versatility lies in its ability to apply reasoning and adaptative capabilities to a wide range of tasks and environments, making these systems highly flexible and robust solutions for complex, real-world applications (Iqbal *et al*., 2026).

2.2 THE AGENTIC AI REVOLUTION IN THE CHEMICAL INDUSTRY: TOWARD TOTAL AUTONOMY

Until a couple of years ago, the chemical industry primary utilized AI as a tool for consultation or prediction (Generative and Analytical AI). An engineer would ask a model to predict the viscosity of a mixture or generate a safety report. However, 2026 marks the year when AI takes action; that is, the industry has transitioned from Generative AI to Agentic AI. This latest class of AI refers to artificial intelligence systems that do not merely process information or predict outcomes but instead possess the capacity to act autonomously to achieve a specific objective (Boskabadi *et al*., 2025; Kumar *et al*., 2026).

Unlike a passive language model (such as a chatbot) that waits for an instruction to respond, the focus has shifted toward AI Agents. An Autonomous Chemical AI Agent possesses the capacity to (Allmendinger *et al*., 2026):

- *Plan:* It breaks down a complex goal into logical steps.
- *Use Tools:* It can access databases, run simulators (such as Aspen HYSYS), or control robotic arms.
- *Reason and Self-Correct:* If an experiment or process fails, it analyzes the 'why' and adjusts its next action without being prompted by a human.
- *Maintain Memory:* It learns from each iteration, improving its efficiency over time.

To draw an analogy: Traditional AI is like a cookbook that tells you what to do; Agentic AI is like an Executive Chef who decides the menu, buys the ingredients, cooks, and adjusts the salt if they notice something went wrong.

Within the framework of Chemical Engineering 5.0—where the goals are radical sustainability and human-machine collaboration—Agentic AI is fundamental for three reasons:

a) Complexity Management (Sustainability)

Sustainable chemical process (such as biomass utilization or CO_2 capture) are significantly more unstable than traditional petrochemical ones. Agentic AI can manage thousands of variables in real-time to maintain the efficiency of a "green" plant that relies on intermittent renewable energy (solar/wind)—a task that exceeds human reaction capacity.

b) The Engineer as an "Orchestra Conductor"

In chemical Engineering 5.0, humans should not be mere screen monitors. Agentic AI handles critical operational tasks (valve adjustments, purity control, prescriptive maintenance), allowing the chemical engineer to focus on strategy, ethics, and innovation. It is a relationship built on trust where the agent proposes and executes, while the human sets the safety boundaries.

c) R&D Acceleration (Autonomous Discovery)

Chemical Industry 5.0 requires new material (batteries, bioplastics). AI agents operate so-called "Self-Driving Labs," where they design and test new molecules 24/7, reducing discovery timelines from decades to months.

2.3 AGENTIC AI IN THE CHEMICAL INDUSTRY

Traditionally, finding a new catalyst took years of trial and error. Today, AI agents utilize Reinforcement Learning to explore chemical space. The agent selects molecular candidates, coordinates synthesis via microfluidics, and analyzes results through automated infrared spectroscopy. This cycle has reduced the time-to-market for new chemical additives by 70-80% (Dana, 2026).

In industries such as paints, cosmetics, or lubricants, agents adjust component ratios in real time to comply with changing environmental regulations, optimizing not only product performance but also its carbon footprint (Iqbal *et al*., 2025).

In industrial complexes like petrochemical plants, interconnected AI agents can manage the exchange of byproducts between facilities owned by different entities. An agent can detect "waste" heat or steam from an ethylene plant and redirect it as "input" for a neighboring facility, optimizing energy at a regional scale.

With plants operated by autonomous agents, cybersecurity becomes a matter of national security. The industry has adopted Zero Trust architecture, where every decision made by an agent must be cryptographically validated to prevent sabotage that could lead to environmental disasters.

In the production phase, Agentic AI has evolved traditional process control systems (PID and APC) into Continuous Operation Agents. Since modern chemical plants are massively interconnected systems, a temperature change in a reactor can affect a distillation column three stages downstream. AI agents monitor thousands of sensors simultaneously and, instead of merely triggering an alarm, they make autonomous corrective decisions:

- Identify a deviation in purity.
- Evaluate the economic impact of adjusting flow versus increasing temperature.
- Execute the change un the valves.
- Generate a technical report explaining the logic behind the decision for the engineering team.

Ai agents now interact with inventory and logistics systems. If they detect that a compressor is operating outside its normal parameters, the agent can:

- Reduce the equipment's workload to extend its service life.
- Check the availability of spare parts in the warehouse.
- Automatically schedule the human maintenance team through digital work orders.

In Mexico and across the globe, the pressure for decarbonization has turned AI agents into critical tools for the Circular Economy (Stahel, 2019). AI agents are capable of performing instantaneous Life Cycle Assessments (LCA) during the design phase. If a chemical engineer proposes a solvent that is efficient but difficult to recycle, the agent suggests alternatives with a higher 'circularity score,' balancing cost, efficiency, and recyclability (Deng & Huo, 2026).

2.4 The New Profile of the Chemical Engineer and the Ethics of Autonomy

The implementation of Agentic AI does not displace the engineer; instead, it redefines their role. By 2026, the chemical engineer no longer spend time on routine material balance calculations or monitoring control screens. Their function is now:

- Defining "Reward Functions": Establishing the ethical, safety, and economic boundaries within which the AI agent is permitted to operate.
- Data Curation: Ensuring that the data used to train the agents is of high level of loyalty.
- Critical Oversights: Intervening in the event of "Black Swan" scenarios (unforeseen situations that the AI has not previously encountered).

Figure 2

Industry 5.0. Human-AI Collaborative and Sustainable Industrial Ecosystems

Source: From the authors by means of artificial intelligence

3 RESULTS AND DISCUSSION

3.1 CASE STUDY: AUTONOMOUS OPTIMIZATION OF A DISTILLATION COLUMN

Let us focus this case study on how Agentic AI transforms one of the most common yet energy-intensive unit operations in the Mexican chemical industry (such as in the Dos Bocas or Minatitlan refineries): the fractional distillation of hydrocarbons (Figure 3).

Figure 3

Digital Twin–Assisted Autonomous Control of a Fractional Distillation Column in Industry 5.0

Source: From the authors by means of artificial intelligence

In a traditional setup, an operator adjusts the reflux and thermal load based on laboratory analyses that take hours to complete. In 2026, a Process Control AI Agent operates as follows:

1). The Scenario: Critical Variability

The distillation column separates a mixture of benzene, toluene, and xylene. The current challenges are:

- Feedstock Composition: The composition of the feed (crude) is constantly changing.
- Energy Costs: The cost of electricity and gas fluctuates according to the time of day.
- Purity Requirements: A purity of 99.9% is required for the benzene stream.

2). How the AI Agent Acts (Step-by-step)

A. Perception and Dat Fusion (Sensing)

The agent does not just "read" the temperature of tray 15; it utilizes Soft Sensors. If a physical sensor fails or experiences fouling, the agent uses a neural network to infer the actual composition based on the pressure and flow of adjacent trays, maintaining operations without shutting down the plant.

B. Reasoning and "Shadow" Simulation

Before moving a valve, the agent runs thousands of simulations on a Digital Twin within milliseconds.

- *Agent's Query:* "What happens if I increase the reflux rate by 5% to compensate for this impurity spike?"
- *Simulation:* "You will improve purity, but the steam consumption in the reboiler will rise by 12%, exceeding today's carbon budget."
- *Decision:* The agent opts for a minor adjustment in the column pressure, achieving the required purity with only 2% increase in energy consumption.

C. Execution and Learning (Action)

The agent directly adjusts the control valves. If the result differs slightly from the simulation (due to undetected fouling within the column), the agent updates it own thermodynamic model. This is "Agentic AI": the system learns from its own errors an adjusts its strategy for the following hour.

4 CONCLUSION

The future of Chemical Engineering 5.0 is autonomous, representing the natural evolution of digitalization toward a model where technology and human ingenuity collaborate seamlessly. Agentic AI is enabling the chemical industry to respond with unprecedented speed to global crises (climate change, pandemics, resource scarcity), prioritizing sustainability, resilience, and worker well-being. Under this Framework, chemical processes do not merely seek maximum profitability; they are designed under the principles of circular economy and carbon neutrality, utilizing technologies such as Digital Twins and AI to personalize production and minimize environmental impact in real-time. In Mexico, the importance of implementing Agentic AI in the industrial sector is critical for competitive survival in the 21st century; adopting these technologies is the only way for national plants to remain competitive against highly automated production centers in Asia and Europe.

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