Ingeniería y Competitividad
Vol 28 (3) 2026 doi: 10.25100/iyc.v28i3.16087

Vol 28 (3)

ISSN
0123-3033
e- 2027-8284

Letter Editor

Data science, machine learning, and artificial intelligence in Chemical Engineering

Ciencia de datos, aprendizaje automático e inteligencia artificial en Ingeniería Química

Diego Ramírez-Malule[1-2] David Gómez-Ríos[1] Howard Ramírez-Malule[1]

[1]Universidad del Valle. Facultad de Ingeniería. Escuela de Ingeniería Química, Cali, Colombia.
[2] Pontificia Universidad Católica de Chile. Programa de Maestría en Ciencia de Datos. Santiago,Chile.

Dear Editor,

Data science, machine learning, and artificial intelligence have permeated all fields of knowledge, and chemical engineering is no exception (1-3) Figure 1 shows the evolution of the scientific outputs of those tools over time based on the retrieved information from the Scopus database. 13,149, 579,813, and 343,007 research articles were found for data science, machine learning, and artificial intelligence, respectively, with no exclusion criteria applied in the query. The first records related to data science date back to the mid-1980s, while records for machine learning and artificial intelligence date back to the late 1950s and early 1960s. Since publications during the first four decades were low compared to the current trend, Figure 1 shows only results starting in 2000.

When all mentioned tools were joined using the Boolean connector "OR", 850,368 records were retrieved, of which 37,889 were related to chemical engineering. These studies date back to the late 1960s. Furthermore, China, the United States, India, South Korea, and the United Kingdom are the leading countries in scientific outputs of these tools related to chemical engineering. Besides chemical engineering, computer science, materials science, and chemistry stand out as the most prominent subject areas (4)

The evolution of those tools, including their applications to chemical engineering, has shown a clear increase since 2017 (Figure 1).

How to cite?

Ramírez-Malule D, Gómez-Ríos D, Ramírez-Malule H. Data science, machine learning, and artificial intelligence in Chemical Engineering. Ingeniería y Competitividad, 2026, 28(3) e-20416087

https://doi.org/10.25100/iyc.v28i3.16087

Received: 15/08/26
Reviewed: 02/09/26
Accepted: 15/09/26
Online: 15/09/26

Correspondence
howard.ramirez@correounivalle.edu.co

Spanish version

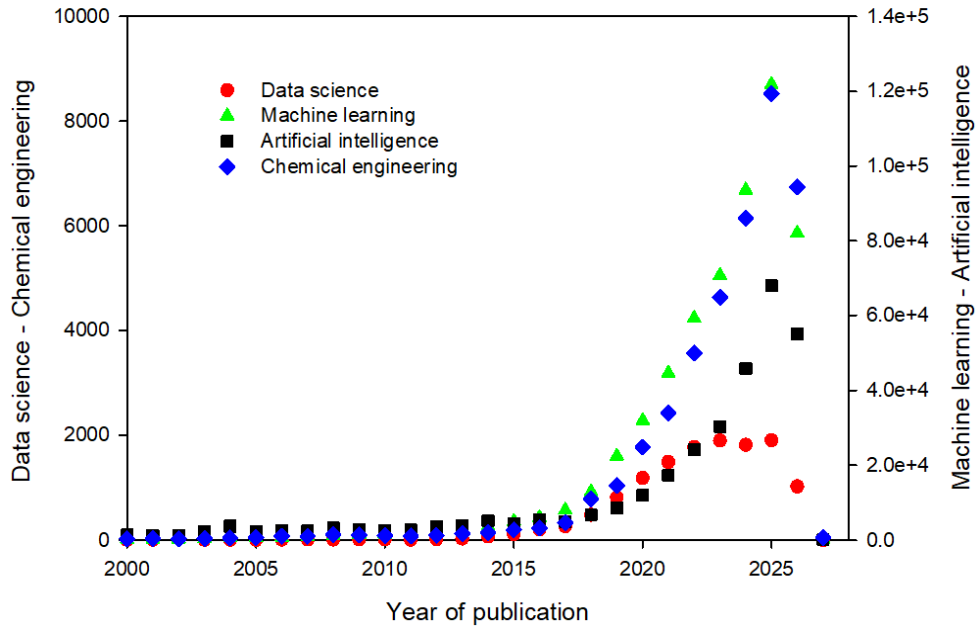

Figure 1. Evolution of the number of research papers related to data science, machine learning, and artificial intelligence, indexed in the Scopus database. Only research articles were considered.

Figure 2 shows a co-occurrence network of the authors´ keywords using VOSviewer version 1.6.20 (5) Here, deep learning, artificial neural networks, optimization, multi-objective optimization, molecular dynamics, adsorption, density functional theory, data augmentation, among others, are the topics that the chemical engineering field is focused on. Additionally, the high-density interconnections of the forty-two nodes among the six clusters indicate a highly multi-interdisciplinary research landscape.

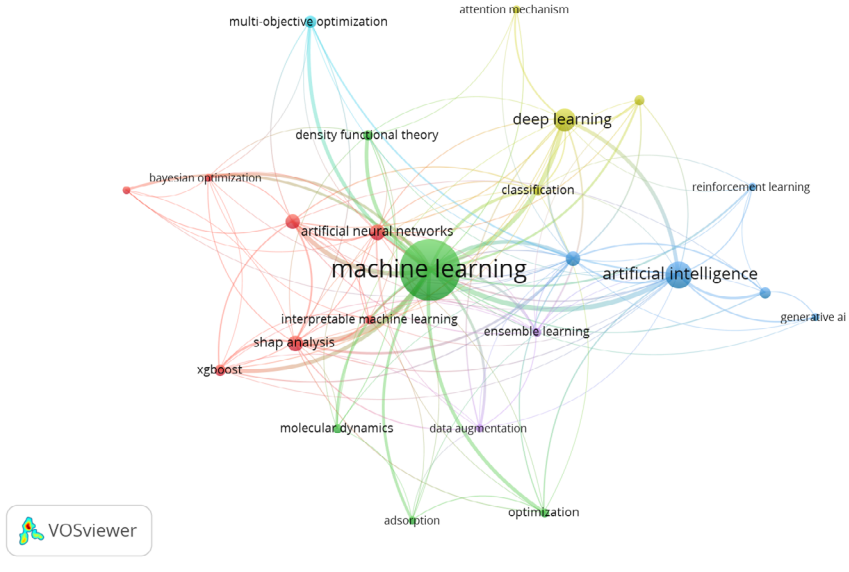

Figure 2. Co-occurrence network of the authors´ keywords. The number of occurrences is 28. The newest 5000 research articles were considered.

doi: 10.25100/iyc.v28i2.16087

Indeed, there are several textbooks available for teaching chemical engineering concepts using the previously mentioned tools. This demonstrates that chemical engineering is incorporating these tools into the current teaching of chemical and biochemical (6-7,1). The topics covered in these texts include: Machine learning in chemical processes; Machine learning in supply chain management; Machine learning in energy integration; Machine learning in time series forecasting; Machine learning in optimal water management in the exploitation of unconventional fossil fuels; Artificial intelligence in chemical engineering data acquisition and integration; Predictive modeling and process optimization in chemical engineering; Artificial intelligence in chemical engineering and process technologies; Artificial intelligence in chemical reaction engineering; Artificial intelligence in chemical kinetics and reactor design; Artificial intelligence in heat and mass transfer in chemical engineering processes; Artificial intelligence in fluid dynamics and multiphase flow systems; Monitoring, Control, and Safety; Real-time decision support systems in chemical and process engineering; Artificial intelligence in quality control and product development; Artificial intelligence in process safety and risk management; Artificial intelligence in sustainable manufacturing and chemical processes; Artificial intelligence in sustainable and smart agrochemicals; Artificial intelligence in energy optimization and renewable energy system integration; AI-enhanced supply chain management in chemical engineering; Artificial intelligence in chemical engineering and applied sciences education; Artificial intelligence for regulatory compliance in chemical engineering industries; Human-AI collaboration in chemical engineering; Regulatory compliance and ethical considerations in integration artificial intelligence (8-9). In summary, they cover a broad spectrum of chemical engineering.

The most productive role of these tools may not be to replace mechanistic chemical engineering knowledge, but to combine it with data-driven learning. Hybrid or phenomenological models can incorporate conservation laws and process knowledge while leveraging experimental and plant data, thereby improving extrapolation, interpretability, and trust compared with purely data-driven approaches. This integration requires chemical engineers to have a solid basis for constructing and understanding phenomenological models in addition to data quality assessment and model validation, since those competences are needed to critically interact with AI-based systems rather than use them as black boxes (1-3).

Based on the previous information, the teaching of chemical engineering and the processes in which it is applied will undoubtedly change in the short and medium term (6,7,1). Process and product design, safety, sustainability, and profitability, among others, will be approached using traditional methods alongside these tools (1-3). But in the medium term, (bio)processes will be addressed more through these tools, and while traditional methods will not disappear, their use will gradually decline. Nevertheless, ethical challenges and concerns associated with data science, machine learning, and artificial intelligence in chemical engineering need to be considered as a key factor for their implementation (1-3).

doi: 10.25100/iyc.v28i2.16087

Conflict of interest statement

None.

Funding sources

None.

References

1. Chew JW, Andersson R, Bierweiler T, Ryttestal P, Wik T. AI in chemical engineering: from promise to practice. AIChE J. 2026;72(7). https://doi.org/10.1002/aic.70358

2. Chiang LH, Braun B, Wang Z, Castillo I. Towards artificial intelligence at scale in the chemical industry. AIChE J. 2022;68(6). https://doi.org/10.1002/aic.17644

3. Schweidtmann AM, Esche E, Fischer A, Kloft M, Repke J, Sager S, Mitsos A. Machine learning in chemical engineering: a perspective. Chem Ing Tech. 2021;93(12):2029-2039. https://doi.org/10.1002/cite.202100083

4.Ramírez Malule HD, Ascencio-Galván ML, Gómez Ríos DA. Bibliometric analysis: a powerful tool for supporting research in engineering. Ingeniería y Competitividad. 2023;25(1). https://doi.org/10.25100/iyc.v25i1.12437

5. Van Eck NJ, Waltman L. Software survey: VOSviewer, a computer program for bibliometric mapping. Scientometrics. 2010;84(2):523-538. https://doi.org/10.1007/s11192-009-0146-3

6. Caccavale F, Gargalo CL, Gernaey KV, Krühne U. Towards Education 4.0: the role of large language models as virtual tutors in chemical engineering. Educ Chem Eng. 2024;49:1-11. https://doi.org/10.1016/j.ece.2024.07.002

7. Keith M, Keiller E, Windows-Yule C, Kings I, Robbins P. Harnessing generative AI in chemical engineering education: implementation and evaluation of the large language model ChatGPT v3.5. Educ Chem Eng. 2025;51:20-33. https://doi.org/10.1016/j.ece.2025.01.002

8. López-Flores FJ, et al. Machine learning tools for chemical engineering. 1st ed. Elsevier; 2025.

9. Sher F, et al. Artificial intelligence in chemical engineering. Sher F, editor. Elsevier; 2026. https://doi.org/10.1016/C2024-0-01393-8