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Artificial Intelligence, Machine Learning, And Data-Driven Methods in Chemical Engineering Education

[1] ALIKORNWO, T.A[2]KikileMasomese,[3]FutugheToju, [4] Paul Uduoghoyo, [5] Miko Haruna, [6]Mfonobong Amadi
[1, 2, 3,4,5,6] *Department of ChemicalEngineering, Faculty of Engineering,University of Port Harcourt, Nigeria.*

Abstract
Chemical engineering education is being transformed by artificial intelligence (AI), machine learning (ML), and data-driven methods as process industries increasingly adopt digital technologies such as industrial internet of things (IIoT), digital twins, advanced process monitoring, and computational modelling. This paper examines the integration of these technologies into chemical engineering education, with emphasis on curriculum development, process simulation, laboratory practice, process systems engineering, and research-oriented skill development. The review shows that AI and ML can support the interpretation of complex process behaviour, predictive modelling, fault detection, soft sensing, process optimization, and analysis of realistic industrial datasets. However, effective implementation requires attention to academic integrity, faculty readiness, computational infrastructure, model interpretability, and the risk of excessive dependence on AI-generated outputs. An integrated educational approach is therefore recommended in which AI and ML complement, rather than replace, fundamental chemical engineering principles.
Keywords—*Artificial intelligence; machine learning; chemical engineering education; data-driven modelling; process simulation; digital twins; process optimization; generative AI.*

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I. Introduction

Chemical engineering education is increasingly being reshaped by artificial intelligence (AI), machine learning (ML), and data-driven process analysis. The discipline has traditionally relied on strong foundations in thermodynamics, transport phenomena, reaction engineering, separation processes, process control, and process design. These fundamentals remain central, but their application is becoming more computational due to the digital transformation of chemical and process industries. Modern chemical plants operate as highly instrumented systems where reactors, distillation columns, heat exchangers, and separation units continuously generate large volumes of operational data. The rise of Industry 4.0 technologies, including industrial internet of things (IIoT), digital twins, and advanced process monitoring systems, has strengthened the connection between plant data and engineering decision-making (Lee *et al.*, 2018). This shift is directly influencing how chemical engineering is taught and practiced. As a result, chemical engineering education is moving beyond purely analytical and empirical approaches toward integrated training that includes data analytics, computational modelling, and machine learning methods. AI and ML are now being introduced as tools within core chemical engineering courses rather than isolated computational topics. This report examines how AI, machine learning, and data-driven methods are integrated into chemical engineering education, focusing on curriculum structure, process simulation training, laboratory practice, process systems engineering, and research-oriented skill development.

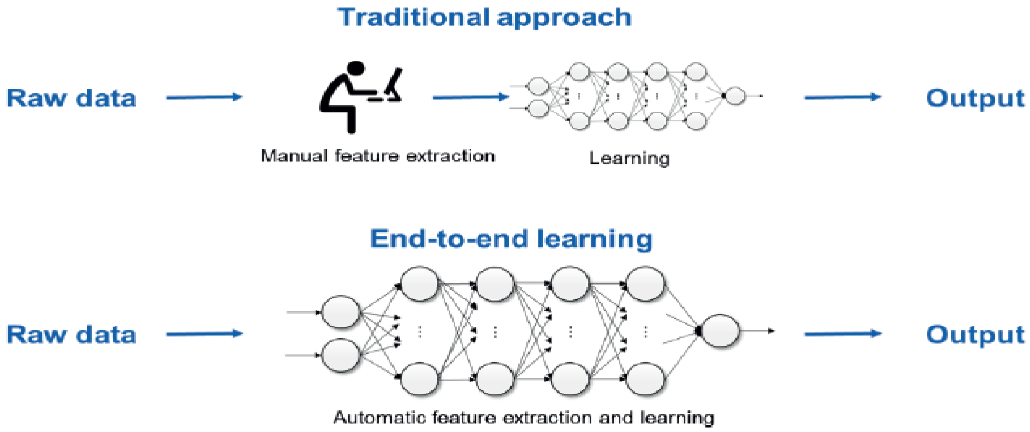

***Figure** 1. Illustration of the concept of end-to-end learning in comparison to manual feature extraction (Schweidtmann et al., 2021).*

In process systems engineering courses, machine learning is used to complement traditional first-principles modelling. Instead of relying solely on mechanistic equations, students learn how data-driven models can capture complex relationships in systems where physical modelling becomes difficult or computationally expensive.Typical applications in chemical engineering education include:

I. modelling and optimization of chemical reactors
II. prediction of separation unit performance
III. fault detection in process equipment
IV. development of soft sensors for unmeasured variables
V. process optimization using historical plant data

Several institutions have introduced structured AI and ML courses for chemical engineers. These courses combine theoretical foundations with practical applications using real or simulated process datasets, enabling students to build predictive models for engineering systems (Vitali *et al*., 2023).

Programming tools such as Python, MATLAB, and R are widely used in training students to pre-process data, train models, evaluate performance, and interpret results in chemical engineering contexts. Importantly, students are trained to combine ML methods with chemical engineering principles such as mass and energy balances, ensuring physically meaningful predictions.

Digital twins are also becoming relevant in chemical engineering education. These virtual process models replicate real chemical systems and continuously update using operational data. They allow students to study process dynamics, evaluate control strategies, and explore optimization scenarios in a safe computational environment (Lee *et al*., 2018).

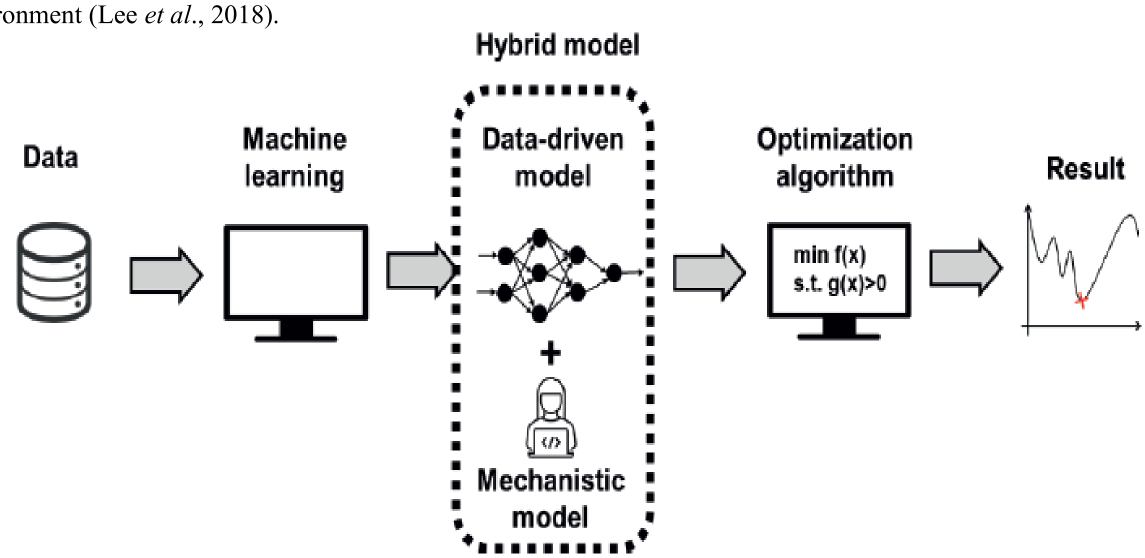

***Figure 2.** Illustration of the data-driven modelling and optimization approach (McBride and Sundmache, 2019).*

The growing availability of industrial process data has accelerated the integration of artificial intelligence (AI) and machine learning (ML) into chemical engineering education. In contrast to first-principles modelling, which depends on mechanistic relationships, ML methods learn directly from data and are commonly applied to prediction, classification, optimisation, and fault diagnosis. This shift aligns with industrial practice where data-driven tools are increasingly embedded in process monitoring and decision-support systems.

Zawacki-Richter *et al*. (2019) applied machine learning models for fault diagnosis in chemical engineering education, offering students hands-on exposure to predictive analytics, causation modeling, and process safety, bridging classroom theory with industrial practice. While Thebelt*et al*. (2022) emphasized incorporating AI tools, adaptive learning platforms, virtual labs, intelligent tutoring systems, and automated assessments into chemical engineering curricula, enhancing personalized instruction and preparing students for Industry 4.0 challenges.

Wu *et al*. (2023) report the development of a dedicated AI course for chemical engineering students showing that core ML concepts such as predictive modelling and optimisation can be effectively introduced within an engineering curriculum. Their work emphasizes that AI is most effective when positioned as a complement to traditional chemical engineering reasoning rather than a replacement for it.

Lavor *et al*. (2024) further demonstrate the value of experiential learning through hands-on ML activities. Their study shows that working with regression, classification, clustering, and neural network models improves students' ability to interpret industrial datasets. A key observation is that exposure to real process data, characterized by noise, missing values, and variability, helps students develop more realistic modelling intuition compared to idealised academic examples.

Schweidtmann (2024) extends the discussion to generative AI, highlighting its growing influence on how engineering knowledge is produced and applied. The work frames AI not only as a computational tool but also as a factor reshaping engineering workflows and problem-solving approaches, with implications for how future engineers are trained.

Keith *et al*. (2025) examines the classroom use of ChatGPT in chemical engineering education. Their findings indicate that students commonly use large language models for coding support, concept clarification, and report preparation. However, the study also notes a limitation: some students rely on generated outputs without adequate verification, which may weaken conceptual understanding.

Cunningham *et al*. (2026) provide a complementary perspective by comparing staff and student attitudes toward generative AI. While students generally view these tools as helpful for learning and efficiency, staff express concerns about reliability, academic integrity, and reduced critical thinking. The study highlights the need for structured AI literacy to ensure responsible use.

Overall, the literature suggests a clear convergence of ML, data-driven methods, and generative AI in chemical engineering education. The strongest outcomes occur when these tools are integrated into authentic engineering problems where they support rather than replace core disciplinary understanding

II. MATERIALS AND METHOD

The study was developed as a literature-based review of the application of artificial intelligence, machine learning, and data-driven methods in chemical engineering education. The materials considered were published studies and scholarly sources addressing AI in higher education, machine learning in chemical engineering, process data analysis, generative AI, digital twins, and experiential learning. The reviewed literature was organized into four analytical areas: AI applications in chemical engineering education; machine learning applications and computational training; data-driven methods and digital-twin applications; and research applications, benefits, challenges, and future directions. Mathematical relationships were included to represent common data-driven modelling and process-learning concepts discussed in the reviewed literature.

Dynamic process equation:

$$dx/dt = f(x, u, \theta) \qquad (1)$$

where:

x = state variable of the process, such as temperature, pressure, concentration, or flow rate.

t = time.

Dx/dt = rate of change of the state variable with respect to time.

U = input or control variable, such as feed rate, heating rate, cooling rate, or valve position.

ɵ= model parameters or physical properties of the process.

f = mathematical function describing how the process behaves

PROCESS OUTPUT EQUATION

The process output equation is given as: $y = g(x, u, \theta)$" (2)

Where;

y = measured or observed output of the process.

x = internal state of the process.

u = process input/control variable.

ɵ = process parameters.
g= mathematical relationship that converts the process state and inputs into the observed output.ɵ

III. RESULTS AND DISCUSSIONS

3.1 AI Applications in Chemical Engineering Education

AI is increasingly used to support the teaching of core chemical engineering subjects by enhancing the interpretation of complex process systems. AI-based learning tools assist students in linking mathematical equations to real process behaviour through interactive simulations and adaptive explanations.

In process control education, AI-assisted tools can visualize dynamic system behaviour and help students understand feedback control, stability, and transient responses. In laboratory-based courses, AI systems support interpretation of experimental data from unit operations such as distillation columns and heat exchangers.

Generative AI tools are also used for process modelling, simulation scripting, concept clarification, and report preparation. Their outputs require validation against physical principles such as conservation laws and thermodynamic consistency.

3.2 Machine Learning Applications

Machine learning has become an important component of chemical engineering curricula because of its increasing use in industrial process modelling and optimization. Students are introduced to supervised learning, unsupervised learning, regression, classification, clustering, and neural networks.

Applications include modelling and optimization of chemical reactors, prediction of separation-unit performance, fault detection, soft sensors, and process optimization using historical plant data.

Python, MATLAB, and R provide practical environments for data preprocessing, model training, evaluation, and interpretation. ML methods can complement first-principles models where complex nonlinear relationships are difficult or computationally expensive to represent.

3.3 Data-Driven Methods and Digital Twins

Modern process industries generate continuous datasets from sensors, control systems, and process historians. Students can therefore be exposed to data preprocessing, statistical analysis, visualization, multivariate analysis, feature extraction, and predictive modelling.

Digital twins provide a further learning environment in which virtual process models represent real chemical systems and can be updated using operational data. They allow students to investigate process dynamics, control strategies, and optimization scenarios in a computationally safe environment.

3.4 AI and ML in Chemical Engineering Research

AI and machine learning are increasingly applied to catalyst development, polymer engineering, chemical product development, carbon capture, hydrogen production, battery and energy-storage materials, wastewater treatment, biochemical processes, and sustainable fuels. These applications influence chemical engineering education by providing research-oriented problems through which students develop computational and analytical skills.

3.5 Benefits, Challenges and Future Directions

AI and data-driven learning can improve understanding of complex process behaviour, support personalized learning, and develop industry-relevant competencies in predictive modelling, process analytics, digital twins, and process optimization.

Important challenges include academic integrity, faculty readiness, infrastructure limitations, model interpretability, and overdependence on AI tools. Future education is expected to integrate AI and data-driven methods more deeply into thermodynamics, reaction engineering, process simulation, process control, and laboratory training.

IV. CONCLUSION AND RECOMMENDATION

4.0CONCLUSION

AI, machine learning, and data-driven methods are significantly transforming chemical engineering education by changing how core concepts are taught, how laboratory training is conducted, and how students engage with process systems.

The reviewed literature demonstrates that these technologies can enhance understanding of complex chemical processes, support realistic data-driven learning, and prepare students for modern industrial environments. However, successful integration requires a balance between computational tools and fundamental engineering principles.

Future chemical engineers will increasingly operate in environments where classical engineering knowledge is combined with AI and machine learning to design, optimize, monitor, and control complex chemical processes.

4.1Recommendation

• Incorporate AI/ML courses and data analytics modules alongside traditional chemical engineering courses.

• Provide workshops and resources so educators can confidently teach and apply AI-driven methods in laboratories, simulations, and research projects.

• Partner with chemical companies to provide students with hands-on experience using real-world process data and smart process technologies.

• Integrate AI, machine learning, and data analytics into chemical engineering research activities

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