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## Editorial: Smart manufacturing: advances and applications of artificial intelligence, machine learning and industrial internet of things in the chemical and biochemical industry

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#### Editorial on the Research Topic

Smart manufacturing: advances and applications of artificial intelligence, machine learning and industrial internet of things in the chemical and biochemical industry

## Introduction

Terms like Smart Manufacturing, Industry 4.0 and Digital Transformation are now commonplace and reflect the increased importance of these technologies in the chemical and biochemical industry, and in the manufacturing sector in general. While advanced digital technologies have evolved over the last few decades in key manufacturing areas, smart manufacturing is still in its early stages and has the potential to significantly improve various manufacturing and biomanufacturing processes in terms of profitability and sustainability. In particular, Smart Manufacturing is expected to contribute substantially to achieving net-zero emissions by 2050, the target set by the Paris Agreement.

Smart Manufacturing is, in simple terms, the use of technologies and processes that maximize data and connectedness to optimize safety, reliability and efficiency in the process industries (Soroush et al., 2020). While there are many advanced technologies that fall under the umbrella of Smart Manufacturing, Artificial Intelligence (AI), Machine Learning (ML) and Industrial Internet of Things (IIoT) have drawn the most research attention and contributed most to the field, to the extent that they are now some of the pillars of Smart Manufacturing/Industry 4.0.

For example, by utilizing AI and ML, data can be analyzed in real-time, allowing for rapid decision-making and optimization. ML algorithms can utilize data collected over time

to predict values and to provide early indications of abnormal process conditions—before critical quality attributes are off specification. Using IIoT connected to machines and equipment, real-time monitoring and control of critical parameters can enable corrective actions before a process deviation can cause equipment failure (Naqvi et al., 2020). According to Sashikumar et al. (2020), a significant reduction in downtime and an increase in productivity have been observed thanks to the usage of these technologies.

This Research Topic aims to highlight the state-of-the-art research in multiple aspects of Smart Manufacturing, including AI, ML, and IIoT and their industrial applications, as well as to provide reviews and perspectives on the topic.

# Overview of the articles featured in this Research Topic

The four contributed papers of this Research Topic demonstrate how AI, ML, and IIoT technologies can improve the performance, safety, productivity, reliability, and sustainability of the chemical and biochemical industry. In the following, their main contributions are highlighted.

Fajardo Muñoz et al. demonstrate how a multi-layer perceptron (MLP) artificial neural network (ANN) can be used to accurately model the relationship between the chemical extraction output from essential oil steam distillation processes and orange peel mass loading. The identified ML model can capture the nonlinear behavior when the process is scaled up. Their contribution provides a viable method to address the scalability issue of citrus essential oils.

Martinetz et al. present an interpretable ML model to gain a better understanding of the solubilization processes of inclusion bodies. Through ML, a reciprocal correlation between protein yield and total protein concentration was identified, together with other findings. The ML results guided the development of an analytic expression, which reflects the fundamental knowledge and properties of the process. The findings from this work highlight the benefits of explainable ML approaches in helping understand certain steps in biopharmaceutical manufacturing processes that are difficult to obtain through the first principal methods.

Wang et al. investigate the molecular design of redox-active materials with higher solubility and greater redox potential window. These properties are instrumental in enhancing the performance of redox flow batteries (RFBs), which have potential applications in storing distributed green energy such as wind and solar power. The authors propose a computational procedure for systematically evaluating organic redox-active species by combining ML, quantum-mechanical, and classical density functional theory calculations. The computational procedure was able to reproduce experimentally observed high-performance cathode electrolyte materials and identify new electrolytes for RFBs by screening 100,000 di-substituted quinone molecules, the largest library of redox-active quinone molecules ever investigated. Lou et al. review various contributions and applications in the field of IIoT and advanced data analytics for environmental and process monitoring. The connected plant concept that uses sensors and digital assets to collect large amounts of data, and then utilizes such data for monitoring and process control to improve plant efficiency, safety, sustainability and asset reliability is also discussed. An example showing existing challenges and research needs in sensor placement is demonstrated. They also present and discuss the future directions in technology, hardware, regulation, cybersecurity, and applications in the IIoT field.

# Concluding remarks and future perspectives

We believe that this Research Topic of articles is informative to scientists and engineers devoted to the research and development of AI, ML, and IIoT technologies, and to the implementation of these cutting-edge solutions in the manufacturing industries.

As can be seen by the contributions in this Research Topic, AI, ML, and IIoT are providing game-changing benefits to the Chemical and Biochemical Industry, and we expect those benefits to keep expanding. These technologies are driving significant improvements in process efficiency, yield optimization and the development of innovative products. With a combination of these technologies, the Chemical and Biochemical Industry can realize the digital transformation promise and further evolve towards a fully smart, data-driven, autonomous and self-optimizing industry of the future.

### Author contributions

JF-C: Writing-original draft, Writing-review and editing. QH: Writing-original draft, Writing-review and editing. JW: Writing-original draft, Writing-review and editing. HY: Writing-review and editing.

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## Conflict of interest

Author JF-C was employed by Linde.

The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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