frontiers | Frontiers in Sustainability

TYPE Perspective
PUBLISHED 20 July 2023
DOI 10.3389/frsus.2023.1210209

OPEN ACCESS

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RECEIVED 21 April 2023
ACCEPTED 04 July 2023
PUBLISHED 20 July 2023

CITATION
Liu D and Sun N (2023) Prospects of artificial intelligence in the development of sustainable separation processes.
Front. Sustain. 4:1210209.
doi: 10.3389/frsus.2023.1210209

Prospects of artificial intelligence in the development of sustainable separation processes

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Addressing the urgent need for more energy-efficient separation technologies is paramount in reducing energy consumption and lessening environmental impact as we march toward a carbon-neutral society. The rapid progression of AI and its promising applications in separation science presents new, fascinating possibilities. For instance, AI algorithms can forecast the properties of prospective new materials, speeding up the process of sorbent material innovation. With the ability to analyze vast datasets related to processes, machine learning driven by data can enhance operations to reduce energy wastage and improve error detection. The recent rise of Generative Pretrained Transformer models (GPT) has motivated researchers to construct specialized large-scale language models (LLM) based on a comprehensive scientific corpus of papers, reference materials, and knowledge bases. These models are useful tools for facilitating the rapid selection of suitable separation techniques. In this article, we present an exploration of AI's role in promoting sustainable separation processes, covering a concise history of its implementation, potential advantages, inherent limitations, and a vision for its future growth.

KEYWORDS

artificial intelligence (AI), separation process, adsorption technique, membrane technique, extraction technique, separation science and technology

Introduction

Since its release in late 2022, ChatGPT, an autonomous machine-learning system and large language model (LLM) developed by Open AI in San Francisco, CA, USA, has taken the world by storm with its remarkable performance and unparalleled capabilities to produce sophisticated and seemingly intelligent writing after training on a massive data set of text (Hu, 2023). If we consider the history of artificial intelligence (AI), three prominent milestones emerge: Deep Blue's defeat of Garry Kasparov in a chess tournament in 1997, Watson's triumph on the game show "Jeopardy!" in 2011, and AlphaGO's unexpected victory in 2016 (Venkatasubramanian, 2019). The emergence of ChatGPT could be viewed as the fourth milestone, representing the first time that AI technology has become widely available and advanced enough to be perceived and utilized by the public. Despite the ongoing concerns surrounding its usage (Thorp, 2023), the incorporation of machine learning-based AI in the development of new technologies has been imperative (van Dis et al., 2023) and yielded tremendous benefits for over a decade in a variety of fields, such as drug discovery, materials science, and geology (Bergen et al., 2019; Hong et al., 2020; Dara et al., 2022).

The separation process, which involves eliminating impurities from raw materials, separating products and by-products, and purifying water and air effluents, constitutes more than 40% of the energy demand in the chemical process industries (CPI) (Humphrey and Siebert, 1992; Kiss and Smith, 2020). The development of sustainable separation processes plays a pivotal role in achieving economic and environmental sustainability, and AI has the potential to dramatically facilitate this process by addressing the limitations of mechanistic modeling through its ability to learn complex behaviors, enable cost-effective model development, and offer optimization advantages (Li et al., 2021).

This article begins by providing a brief history of using AI in separation. It then delves into AI's potential to drive sustainable separation technologies' development. Finally, the limitations of AI are highlighted, and an outlook for its growth is presented. The goal of this article is to give a comprehensive understanding of AI's role in the advancement of sustainable separation processes.

History of AI in separation process development

In fact, the use of AI to solve separation-related problems is not recent news (Quantrille and Liu, 2012); as early as 1983, researchers from Carnegie Mellon University developed an expert system called CONPHYDE (CONsultant for PHYsical property DEcisions) to predict the physical properties of complex fluid mixtures (Banares-Alcantara et al., 1985). This era is regarded as Phase I: (∼1983 to ∼1995) of AI in chemical engineering (Venkatasubramanian, 2019). In the post-1990 era, a critical transition occurred in artificial intelligence applications, marking the inception of Phase II (∼1990 to ∼2008). This transition involved a shift from the top-down design paradigm employed by expert systems to the bottom-up paradigm embodied by neural networks. The neural network approach possesses the inherent capacity to autonomously derive knowledge from substantial data sets, thereby streamlining the processes of model maintenance and development, and was found to be capable of accurately modeling complex membrane separation processes (Niemi et al., 1995; Bowen et al., 1998a,b). Throughout Phase I and II, spanning two decades of focused endeavors, the implementation of AI has failed to produce the expected transformative outcomes within the realms of separation process development and the broader field of chemical engineering. This may be attributed to various factors, including insufficient data, limited data accessibility, inadequate computational power, and lack of programming environments/paradigms (Schweidtmann et al., 2021). Today, with the emergence of essential technologies represented by convolutional neural nets (CNNs), reinforcement learning, and statistical ML, as well as hardware advances, especially GPU computing, which brings cheap and powerful computing power, the AI application has entered deep learning and the data science era (Venkatasubramanian, 2019). In Phase III (2005–Present), the rise of bottom-up, data-driven strategy for knowledge acquisition and modeling has made it much easier to address more complicated "big data" domain problems. With the technology push and industry pull, AI offers new possibilities to overcome pressing challenges in the traditional separation process (see Figure 1).

Perspective of AI in sustainable separation process development

In 2016, Sholl and Lively identified seven representative chemical separation processes that, if improved, could achieve significant global benefits (Sholl and Lively, 2016). These challenges include separating hydrocarbons from crude oil, uranium from seawater, alkenes from alkanes, greenhouse gases from diluted emissions, rare earth metals from ores, benzene derivatives from each other, and trace contaminants from water. To address those challenges, the traditional separation techniques, such as multistage distillation and differential temperature adsorption, often incur a large carbon footprint and processing costs when employed (Shao, 2020). Developing efficient and low-energy separation technologies independent of liquid phase changes is considered to be the key to reducing carbon emissions in the chemical industry, and AI will contribute to the advancement of sustainable separation technologies in the following ways (see Figure 2).

Physicochemical property prediction of complex mixtures

Knowledge about the physicochemical properties of chemicals and their mixtures is crucial for new separation process design. Complex mixtures, such as lignin depolymerization products, crude and renewable oils, etc., require decomposition into more detailed components before property calculations. Despite the variety of reconstruction methods, it is still difficult to accurately calculate the properties of mixtures, such as boiling point, density, and viscosity (Deniz et al., 2018). For certain complex feedstocks, like plastic waste pyrolysis oils containing large amounts of highly reactive olefins, it is almost impossible to experimentally determine the physical properties due to the reactivity of this mixtures (Daothi et al., 2021). Integrating a machine learning approach to correlate the physicochemical properties of mixtures with the molecular properties and molecular structures of individual compounds can potentially obtain more accurate predictions than existing methods (Dobbelaere et al., 2022). And this is of great importance to improve the hydrocarbon separation of crude oils containing many complex molecules, both in terms of developing new technologies and optimizing the operating conditions of existing units.

Membrane technology

Implementing advanced membrane separation technology leads to a more sustainable process that significantly lowers energy consumption and carbon footprint, exceeding the efficiency of traditional distillation methods in separating and purifying many compounds (Sholl and Lively, 2016). However, the challenge of accurately predicting the structure-process-property relationship for the effective design of new membranes with desired properties has impeded the progress of membrane technology. This is attributed to the high dimensional features in membrane design, including intrinsic information like chemical structure, pore size,

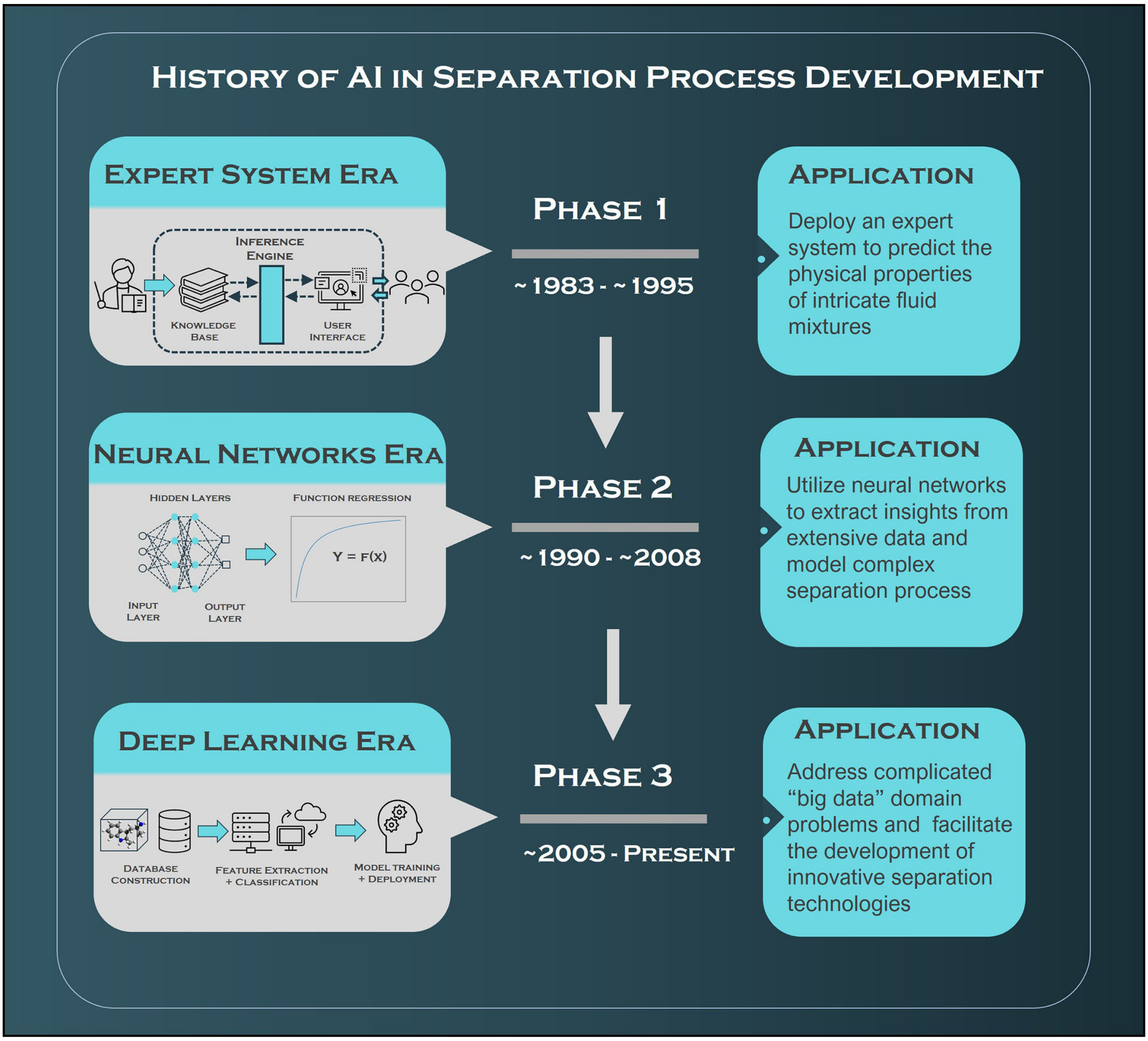

FIGURE 1
History of AI in separation process development.

and surface area, extrinsic conditions like reaction temperature, concentration, and pH, the difficulties posed by the vast design space of potential materials in screening, and the added complexities of physics and chemistry involved in complicated membrane systems (Yin et al., 2022). The remarkable capability of machine learning to process massive and high-dimensional data shows great potential for hastening the advancement of membrane technology at various stages, including membrane design (Barnett et al., 2020; Guan et al., 2022), fabrication (Fetanat et al., 2021; Gao et al., 2021), and operation (Rall et al., 2020). For separating alkenes from alkanes, the membrane technology is considered the most promising approach. However, the current state of the technology is insufficient for bulky separation and necessitates the use of cryogenic distillation for further refinement of the products (Chen et al., 2022). Additionally, scaling up the membrane technology to meet industrial demands, which may require surface areas of up to 1 million square meters, presents a significant challenge that requires new manufacturing methods and advancements in material properties. AI has the potential to play a crucial role in overcoming these hurdles.

Adsorption technology

Adsorption technology is a promising solution for large-scale industrial separations of dilute streams due to its low energy requirements and favorable economics. Over the past two decades, adsorption technology has seen significant growth with the development of new adsorbents and modifications of existing adsorbents in compositions, structures, and functions. The technology has been utilized to address complex separation challenges, such as isomer separation (e.g., xylene, cresol, and

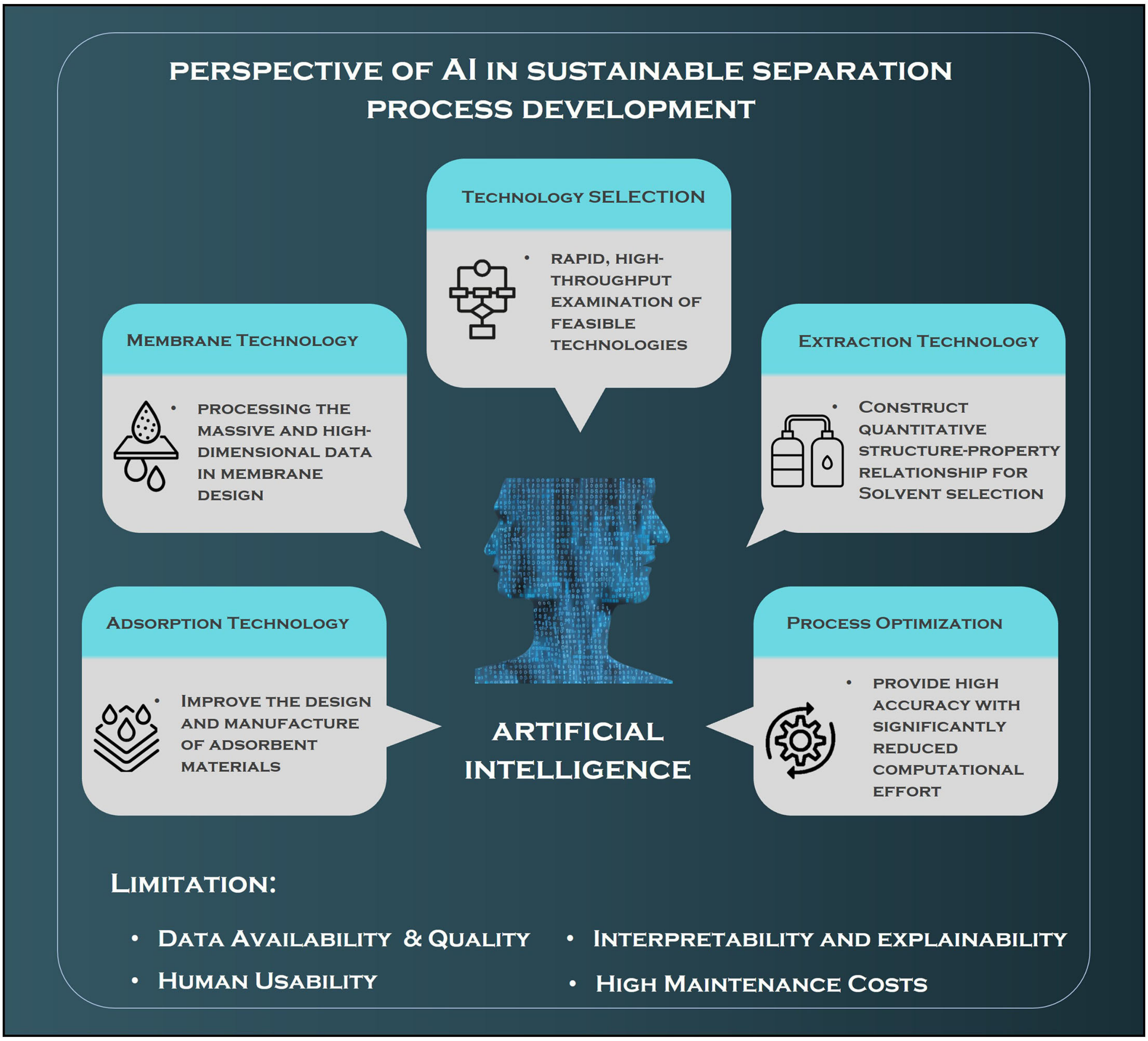

FIGURE 2
Perspective of AI in sustainable separation process development.

toluene), CO_2 capture, water treatment, uranium extraction from seawater, and the recovery of Rare Earth Elements (REEs) (Mandal and Kulkarni, 2011). The integration of AI, such as advanced machine learning algorithms, has the potential to further improve the design and optimization of adsorbent materials. For instance, Metal-Organic Frameworks (MOFs), a newly discovered class of porous crystalline materials composed of multimetallic units and organic linkers, can be functionalized for CO_2 separation, particularly in the removal of CO_2 from CO_2/H_2 (pre-combustion carbon capture), CO_2/CH_4 (natural gas purification), and CO_2/N_2 (post-combustion carbon capture) mixtures (Mandal and Kulkarni, 2011). However, the synthesis of novel MOF structures still necessitates researchers to rely on their expertise and adopt a trial-and-error methodology. Applying machine learning to predict synthesis parameters for a target MOF crystal structure, based on scientific literature and high throughput experimental data, could substantially advance and expedite the chemical synthesis process (Luo et al., 2022). LanM, a protein-based biosorbent, can recover REEs from e-waste and lignite leachates. It has demonstrated exceptional selectivity for lanthanides with over one million times higher than that for other ions (Dong et al., 2021; Ye et al., 2023). However, LanM is currently unable to facilitate the separation of individual lanthanides from one another, necessitating further optimization of protein selectivity to attain this objective. Employing machine-learning-guided directed evolution in protein engineering enables the enhancement of protein functions. Machine-learning methodologies facilitate the prediction of sequence-to-function mapping in a data-driven manner, circumventing the need for comprehensive models of the underlying physical or biological pathways. By learning from the properties of characterized variants, these approaches could expedite directed evolution, utilizing the acquired information to select sequences more likely to exhibit improved properties (Yang et al., 2019).

Extraction technology

Liquid-liquid extraction (LLE), also known as solvent extraction or partitioning, is a widely employed separation technology in numerous scientific and industrial applications. The technique is based on the differential solubility and partitioning of solutes between two immiscible liquid phases, typically one aqueous phase and one organic phase (Cantwell and Losier, 2002). The choice of solvent is critical to the LLE process, as it directly affects the partition coefficient and, consequently, the extraction efficiency. The ideal solvent should possess high selectivity for the target solute, low miscibility with the other phase, low toxicity, and ease of recovery (Gmehling and Schedemann, 2014). Currently, there are two main approaches to solvent selection: the use of experimental thermophysical properties stored in a database for reliable results with limited solvent selection and the use of prediction models or empirical methods for a broader range of solvents with lower accuracy in predicted separation factor (Piccione et al., 2019). In the case of mixed solvent extraction, extensive experiments are often necessary to determine the optimal solvent system. For instance, centrifugal partition chromatography (CPC), an emerging liquid-liquid preparative chromatographic separation technique used in pharmaceutical and natural product purifications, frequently requires a solvent system with three or more components (Lorántfy et al., 2020). When applied to complex feedstocks, such as lignin depolymerization products, multi-stage hybrid solutions with various components are essential to achieve the desired outcomes (Alherech et al., 2021). AI presents considerable potential for enhancing the intricate solvent selection process. The training dataset can be accessed and curated from a myriad of published sources, including academic journals, printed handbooks, and online repositories. Machine learning can be employed to construct quantitative structure-property relationship (QSPR) models, which link the molecular structure of solvents and solutes to their physicochemical properties and extraction performance which predict the behavior of untested solvent-solute combinations, offering insights into the most promising solvents for specific extraction tasks (Kern et al., 2022). Combined with optimization algorithms, AI can facilitate the exploration of multi-dimensional solution spaces and identify optimal trade-offs between competing objectives, such as extraction efficiency, selectivity, environmental impact, and cost.

Process optimization and fault detection

Upon transitioning a high-efficiency separation method from laboratory-scale validation to industrial-scale implementation, the process complexity increases substantially. A simple step performed at the bench scale may result in a unit operation with numerous operating parameters during the scaling-up process. Considering this, developing a comprehensive tool that can effectively simulate and optimize processes to minimize energy losses and optimize separation efficiency is imperative. Even a 1% improvement in energy consumption can result in substantial economic and environmental benefits. The traditional mechanistic-based methods relied on chemical, fluid-mechanic, and thermodynamic laws, which require a deep understanding of the underlying physics. However, this conventional approach is complex and computationally demanding due to the highly nonlinear nature of the process parameters and output.

In contrast, the data-driven machine learning approach could provide a similar level of detail and accuracy as mechanistic-based methods by utilizing readily available process data, with a significantly reduced computational effort (Rahimi et al., 2021). Another process-level area where AI can be highly effective is fault detection and diagnosis (Tian et al., 2020), an application scenario that garnered significant interest from the industry during its early stages (Venkatasubramanian, 2019). The abnormal conditions in separation processes are often masked by factors such as compensatory controls, measurement errors, and operator ignorance. Currently, the primary methods for identifying faults in abnormal operating conditions still rely on human experience, making it difficult to accurately and quickly detect abnormalities, potentially leading to incorrect decisions, improper actions, and even hazardous incidents (Van Hardeveld et al., 2001). By analyzing the complex and nonlinear relationships between processing parameters, machine learning algorithms can improve fault detection by identifying relevant features or combinations of features that indicate abnormal behavior even before it occurs.

Beyond the advancement of specific separation technologies, AI has the potential to make substantial contributions to the resolution of challenges at the system level of separation processes. Selecting suitable separation techniques, for instance, is a complex task requiring meticulous contemplation of various parameters. These include the physical and chemical attributes of the substance undergoing a separation, operational conditions, efficiency, cost, environmental restrictions, and prevailing regulatory standards. Machine learning algorithms can be leveraged to examine these properties of the subject substance and establish correlations with the performance of diverse separation techniques. This potential opens the door to rapid, high-throughput examination of feasible technologies—a process that, in traditional approaches, could be laborious and time-consuming. By integrating AI into the system-level design and decision-making processes, we can therefore expect substantial enhancements in the efficiency and effectiveness of separation system design and operation.

Limitations and outlook

While AI has shown significant promise in revolutionizing various aspects of sustainable separation process development, several limitations must be considered.

Data availability and quality

Knowledge acquisition and modeling using deep convolutional networks, reinforcement learning, and statistical learning are primarily bottom-up, data-driven strategies that require large amounts of data to achieve satisfactory results. This data requirement may not pose a significant challenge for some technologies development, such as adsorbent materials design, zeolite (Baerlocher and McCusker, 2023), and MOF (Groom et al., 2016), which already have extensive databases with comprehensive information that can serve as a training set. As for process-level optimization, data could be achieved by utilizing vast amounts of historical data or through direct simulation using process software. But it should be noted that this field is not exactly a "big data" domain. The data points generated from a complex laboratory separation process are typically at a slow pace and are frequently reported in an inconsistent manner in the literature.

Moreover, due to commercial considerations, some high-value data are kept in the databases of industry companies and may not be readily accessible to the public. To address the data shortage, accelerating the laboratory's automation, promoting high-throughput experimental techniques, and gradually creating a unified data platform for storing and sharing data related to the separation process could be effective solutions. Also, multi-party validation could be utilized to create a high-quality training set, ensuring the removal of incorrect data points and reducing inaccuracies.

Interpretability and explainability

AI models, especially the deep learning models, can be considered "black boxes" due to their complex and inscrutable decision-making process. However, the separation process is governed by fundamental laws and principles of physics, chemistry, and biology. The lack of transparency in AI models may impede the generation and transfer of this fundamental knowledge. This makes it challenging to incorporate domain-specific expertise and principles into the model, which results in suboptimal solutions. Considering the stringent safety requirements of industrial separation processes, the inability to explain AI solutions raises concerns about reliability and complicates the task of meeting regulatory requirements. In the future, AI should aim to create more comprehensive systems that go beyond purely data-driven methods. This can be achieved through the integration of Explainable AI (XAI) techniques such as Local Interpretable Model-agnostic Explanations (LIME) or Shapley Additive Explanations (SHAP) and the use of hybrid models that blend data-driven processing with first principles-based knowledge. This approach will not only enhance the decision-making process but also provide insights into how decisions are made, explain the underlying causes, and allow for specialized knowledge in specific domains.

Human usability

In addition to the advancements in technology, AI presents new challenges to the people who utilize it, particularly in the field of separation technologies. Experts in this field typically come from experimental disciplines, including chemical engineering, chemistry, materials science, and biology. Most have not received systematic training in artificial intelligence during their academic pursuits, although their mathematical, statistical, and programming skills may be helpful in mastering AI technology. As the low-hanging fruit in this field is harvested, gaining a deeper understanding of machine learning, transitioning from merely knowing how to use AI to understand why AI is solving problems in specific ways, will become essential for further progress. Just as process experts should not ignore learning about partial differential equations despite the popularity of commercial process software, mastering the underlying principles of AI is crucial.

Conversely, AI methods tailored to this specific area should be made available to researchers in a more user-friendly and accessible form. There is no need to solve partial differential equations manually when process software can provide solutions in a much easier way. Similarly, offering easy-to-use AI tools can help researchers focus on their core expertise and drive innovation while maintaining a strong human presence in decision-making.

Conclusion

In 1950, when Alan Turing posed the question, "Can machines think?" (Krach et al., 2008), many people considered it a distant dream. However, by 2023, OpenAI's GPT-4 has made remarkable advancements, showcasing its capabilities by passing the bar exam (Katz et al., 2023), outperforming 90% of humans on the SAT (Leswing, 2023), and even persuading skeptics of the rapidly approaching era of AI integration into daily work and study. In fact, the next generation of scientists and engineers is already getting a head start on embracing AI technology, albeit in a way that educators may not appreciate (Nancy Loo, 2023). Separation processes, a field dating back to early civilizations when humans sought to process food and pharmaceutical products, now span all manufacturing industries and account for 22% of all in-plant energy use in the United States (Angelini et al., 2005). Developing novel, high-efficiency separation technologies is crucial for reducing energy consumption and environmental footprint in pursuit of a carbon-neutral society. Rapid advancements in AI and its application in this essential field offer exciting opportunities, such as the better design of sorbent materials, improved selection of extraction solvents, and optimized process operating conditions. By harnessing the power of AI, researchers, and engineers have the potential to revolutionize separation processes, transform industries, and contribute to a more sustainable future.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

DL and NS conceptualized the topic and determined the scope. DL conducted the literature search and drafted the manuscript. NS provided critical insights on the manuscript content and

provided substantial revisions. All authors reviewed and approved the final manuscript.

Funding

The project was funded through BETO's Bioprocessing Separation Consortium.

Acknowledgments

The authors from the ABPDU acknowledge support from the U.S. Department of Energy's Bioenergy Technologies Office (BETO), which is part of the Office of Energy Efficiency and Renewable Energy (EERE), and funding from the American Recovery and Reinvestment Act.

Conflict of interest

The 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.

The handling editor ET declared a past collaboration with the author NS.

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