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Dynamic Of Batch Chemical Processes Using Intelligent Strategies: A Review

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Abstract: Batch reactors are extensively used in chemical industries because of their adaptability and superior product quality; however, their nonlinear and time-varying characteristics present considerable challenges for dynamic modeling and control. Conventional modeling methods frequently inadequately represent intricate behaviors. This review examines the contribution of artificial intelligence (AI) techniques—specifically machine learning (ML), neural networks (NN), and reinforcement learning (RL)—to the improvement of modeling, prediction, and control in batch chemical processes. The primary objective is to assess and compare these AI methodologies, discover their strengths and shortcomings, and underline their value in industrial applications. Principal findings indicate that AI-driven strategies greatly enhance performance, adaptability, and optimization in batch systems. The study addresses challenges including data requirements and computational demands and suggests future directions such as hybrid AI frameworks and real-time optimization. This study seeks to direct researchers and practitioners toward enhanced and effective batch process management.

Keywords: Batch process; Dynamic modelling; Artificial intelligence (AI); Adaptive Neuro-Fuzzy

1. Introduction

Batch processes are widely employed in modern industrial applications because of the rising demand for high-value products, especially within the chemical industry [1]. Their straightforward design, economical production, and operational simplicity make them extensively applicable in pharmaceuticals, semiconductors, food, plastics, polymers, biotechnology, and various other industries [[2],[3],[4],[5],[6]]. The primary aim of batch processing is to optimise the yield of target products while minimising unnecessary by-products, ensuring safety, and enhancing product quality within a limited processing duration [[7],[8]]. In contrast to continuous processes, batch systems provide enhanced operational flexibility [9] ,but encounter significant challenges including nonlinearity, process instability, variability between batches, time-dependent dynamics, and the absence of a stable operating point [[10],[4],[11],[12]]. These challenges complicate model-based optimization and control, frequently necessitating innovative frameworks that address process uncertainties, delays, and fluctuations.[[9],[1]].

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A prime illustration is the batch reactor, which is essential in the production of chemicals, food, and pharmaceuticals. These reactors are enclosed containers in which reactions occur under dynamic conditions, necessitating precise control to adhere to stringent quality [[5],[13]]. In order to improve these systems effectively, researchers use data-driven models and machine learning methods [11]. Since the quality standards for the final products are often quite stringent, effective control is crucial [5]. The issue of quality-related control has also attracted more attention recently, as the results of batch processes often need to be of a fairly high quality. The idea of “quality-related” control - also referred to as “output-related” control - has been put forward [14]. The goals of control include enhancing product concentration, reducing by-products, increasing process output, and enhancing efficiency [15]. Strong economic competition and sustainable development goals, as well as the need to operate the plant more profitably and with higher quality specifications, have also contributed to the development of new technologies capable of operating modern factories in a safe and profitable manner. Process monitoring, estimation and control have gained increasing attention as a result of these factors. Thus, among the technologies associated with process monitoring, process monitoring serves as an important component [16]. In the context of batch recipe optimisation, industrial practices have predominantly relied on trial-and-error methods or experiential learning. The operating recipe is initialised based on the engineer/operator's prior knowledge and experience, and it is subsequently refined as runs are repeated and results are collected. The success and efficiency of this approach are heavily reliant on the individual's level of expertise, which may lead to inconsistent results. Dynamic model-based optimisation, whether conducted off-line or on-line, has been the subject of extensive study and has seen limited industrial application. Nonetheless, the necessity for a comprehensive and precise dynamic model has been the primary obstacle to extensive industrial application, and heuristics-based recipe development continues to be the standard in industrial practice [1]. As the complexity of practical batch processes continues to rise, monitoring methods that rely on the supposition that the process feature is straightforward and ideal are no longer capable of producing reliable and accurate monitoring results [8]. Artificial intelligence has emerged as a new framework in the field of information technology, denoting the ability of machines to perform tasks and functions that reflect human cognition. Techniques such as machine learning, neural networks, fuzzy systems, and genetic algorithms are increasingly being used to address complex practical challenges and are gaining significant traction in contemporary discourse [17]. Artificial intelligence is the process of integrating human thought and behavior into machines or systems. We are now living in a technological era referred to as the Fourth Industrial Revolution, sometimes referred to as Industry 4.0 or (4IR) [18]. Artificial intelligence applies to the development of computers that mimic human cognitive abilities [19]. It also refers to the process of giving machines the same level of intelligence as the human brain [20].The study of artificial intelligence is concerned with how the human brain makes decisions, learns, thinks, and solves problems. The goal of the broad field of artificial intelligence is to build intelligent machines. [21]. There are many researchers who have been studied implementation of artificial intelligence in batch processes. Peres et al [22] conducted a research on detecting batch process faults through the selection of integrated variables with multi-directional principal component analysis, focused on developing a method using Multiway Principal Component Analysis (MPCA) in parallel with variable selection. This approach improves fault detection by identifying the variables that most affect process performance, which helps analyze data more effectively and efficiently, enabling early problem detection and industrial process stability. The research shows how Artificial Intelligence may overcome standard modeling methodologies, particularly for complex, nonlinear, and time-dependent batch reactor system characteristics. The article examines how machine learning (ML), neural networks (NN), deep learning, and reinforcement learning might increase reactor accuracy, prediction, and optimization. This study aims to provide academics and industry researchers a comprehensive grasp of AI-based batch reactor dynamic modeling. Georgakis et al [22] used data-driven modelling to optimise batch operations in complicated, low-production industrial batch processes when knowledge-based models are unavailable. Industrial polymerisation process behaviour is modelled and batch cycle time reduced using dynamic evolutionary design of experiments (DoDE). The cautious strategy chooses beginning experimental circumstances comparable to prior procedures to assure safety. The model is modified to find ideal operating parameters as more data is received, improving efficiency. This adaptive technique optimises batch processes safely and reliably in industrial applications. Yadav et al. [13] utilised open-loop data from a pilot plant reactor to construct an autoregressive model with external inputs (ARX) and nonlinear autoregressive model (NARX) to improve batch reactor process control. Inability to handle nonlinear dynamics causes conventional linear controllers to use too much power and aggressively change variables. The paper suggests a nonlinear predictive controller (NMPC) to smoother responses to controlled variables and reactor temperature, improving control performance. Simulated and real-time trials confirm the technique for batch reactor optimisation. Kurniawan et al [23] builded up a moving batch reactor for degumming crude palm oil with phosphoric acid (H_3PO_4). The study proposes a superior scale-up strategy that uses degumming efficiency (measured by gum concentration) instead of geometric similarity, which fails when reactor geometry is different. CFD velocity distribution and mass transfer modelling was applied to a flat-bottomed moving tank reactor from laboratory studies in a three-necked circular vessel. The bigger reactor's minimum fan speed of 93 rpm mirrored laboratory research' greatest degumming efficiency in simulations. Industrial degumming operations are more predictable and efficient using this procedure, making reactor scale-up more dependable. Yang et al. [24] used advanced monitoring, communication, and computing technologies in the Industrial Internet of Things (IIoT) architecture to analyse smart manufacturing (SM) in the fourth industrial revolution. It shows how high-performance computation and sophisticated modelling improve industrial adaptability. The study shows how data-driven and knowledge-enabled hybrid models (HM) fit developing industrial paradigms in SM.Despite the increasing implementation of artificial intelligence (AI) methodologies in batch chemical processes, a comprehensive review critically analysing and comparing these techniques regarding their efficacy, complexity, and practical applicability remains absent. Most current reviews are either general in scope or restricted to particular applications, lacking a systematic assessment of the strengths, limitations, and future prospects of AI in batch process modelling and control.

This review aims to provide an overview of essential Artificial Intelligence techniques.

1.Employed in batch chemical processes, encompassing modelling, control, and monitoring strategies.
2. Evaluate the strengths and weaknesses of these techniques regarding accuracy, complexity, and industrial applicability.
3. Identify recent case studies that illustrate the tangible effects of Artificial Intelligence on enhancing batch process performance.
4. Identify existing challenges and propose future strategies for the integration of Artificial Intelligence in batch process industries.

2. *Characteristics* and *Modeling Approaches* of Batch Processes

2.1 *Characteristics* of Batch Processes

Batch processes are characterized by their limited duration, unsteady state, and nonlinear properties [25], non-steady operation, nonlinear dynamics, and constraints on the path and endpoint. Cintra et al. [26] explored the challenges of batch process monitoring, which generates time series data with both batch-to-batch variability and serial correlation over time. Traditional approaches rely on multi-way principal component analysis (MPCA) to handle batch variability but often ignore the time series nature of the data. Newer approaches integrate time series models and neural networks to balance sources of variability. This paper presents a model-free approach based on the theory of U-statistics, enabling the development of V-control charts that effectively capture patterns of variability. This new technique enhances batch process monitoring by providing a robust statistical framework without the need for pre-defined models.These problems are often exacerbated by high variability in the quality and condition of the raw materials, as well as other uncertainties in the process (e.g., turbulence, noise, and model errors) [27]. Batch processes exhibit significant nonlinearity in contrast to continuous processes, leading to increased interest in model-based nonlinear control of these systems. Batch process control is commonly used for repetitive chemical reaction tasks. The process begins with precise filling of a liquid material, followed by a controlled reaction that discharges or transfers the quantities of the processed material. The input materials are contained in a vessel reactor and undergo a series of processing activities over a predetermined duration according to the recipe [28]. Luo and Bao [29] studied a sparse knowledge integrated data modelling (KDIS) technique for batch process monitoring to solve the drawbacks of data-driven models that lack interpretability and process knowledge. The KDIS approach improves defect identification and diagnosis by combining process data and expertise. The research presents two novel fault detection monitoring indicators and two-level contribution diagrams that identify defective variables and variable groups connected with control loops or physical/chemical linkages. This method enhances process interpretability and monitoring efficiency, making it useful for industrial batch process optimisation Among the various limitations of batch reactors, safety concerns have significantly hindered their progress . Thermal runaway is a major safety concern for exothermic reactions, contributing to 25% of chemical plant accidents, which may include overpressure, release of materials, fire, or explosion. Thermal runaway has been observed in almost all types of reactors (e.g., batch reactors) [6]. Thermal runaway is one of the dynamic properties of a batch reactor and is a phenomenon that occurs during an exothermic process. The reaction generates heat, which raises the temperature and increases the reaction rate. This will generate high heat, thus causing an additional rise in the reaction temperature, etc. A chemical system is considered to be regulated if the heat generated by the reaction is less than that released by the reactor cooling system. If the heat lost is less than the heat generated by the process, it may lead to thermal runaway .In many sectors of the chemical industry, especially within the fine chemical industries, the majority of synthetic processes are exothermic. The main problem with these responses is the lack of temperature regulation during failure, thermal runaway may occur in this scenario [30].

2.1 *Characteristics* of Batch Processes

Dynamic modeling is a crucial technique for enhancing the learning of complex processes and determining optimal operating conditions for process control [31]. Process modeling and optimization are essential for assessing the economic feasibility of a process. Moreover, creating a mathematical model that encompasses several key processes can reduce process costs, enhance efficiency, and provide comprehensive knowledge of the process. Modeling processes also provide new perspectives and understanding of phenomena, mechanisms, interaction modes, and thermodynamics. Furthermore, these models are useful for predicting performance processes prior to actual operation and testing. Modeling helps in understanding response events and predicting the behavior of the entire system. Therefore, a clear understanding of different models is essential for process optimization, kinetics, scale-up, or process modification [32]. Ishitobi et al. [33] addressed standard PID controllers' inefficiencies, which need human parameter and reference signal tweaking. The paper recommends Model Predictive Control (MPC) to improve optimisation, although it also recognises the difficulty of maintaining several models for diverse product and equipment combinations. The proposed system uses predefined mathematical models for common process parts and experiment-driven models for empirically tuned components for control improvement. Batch process modelling is simplified and automated using this hybrid technique Current industrial processes are often complex and present significant modeling challenges. Accurate mathematical models are essential for process control and optimization, which requires accurate parameter estimation [8]. All modeling methods can be broadly divided into two groups: those based on first principles and those driven by actual evidence. A desirable property of first-principles models is their ability to directly apply physical conservation rules, such as mass or energy balances, to processes, thus capturing their underlying mechanics. However, first-principles models are still not easy to build and update. An alternative that has recently gained popularity is data-driven modeling, which uses a large amount of historical process data. It is possible to build models from process data using any of a number of available modeling methods. When it comes to human-like tasks such as language processing, image recognition, clustering, pattern identification, and classification, neural networks have recently shown impressive results. [34]. The final form of the model depends on why it was created. To help people better understand how things work, models used in operator training simulations can be quite complex. Since computers can perform a lot of calculations quickly, the most important thing here is how accurate the model is. In contrast, the models used to create control systems must be so simple that they can be used in automated control equipment that does not have a lot of computing power. It takes less work to obtain a final control rule when using simple models of mathematical changes. Also, engineers' understanding of the process is often demonstrated in simple models, and controls based on simple models are better for teaching employees about the process. The person in charge of the process must always know why the controller is changing the variable being controlled, and this is especially important for model-based control methods [35].

3 .Artificial Intelligence Methods for Dynamic Modeling

AI-based modelling is the key to making systems that are automatic, smart, and clever that meet the needs of today. Building a good Artificial Intelligence model, on the other hand, is hard because real-world problems and facts are always changing [18]. Artificial Intelligence is divided into machine learning, deep learning, and data analytics. Artificial Intelligence thrives mostly due to its unique ability to learn and modify the system based on prior facts before arriving at a conclusion [36]. Artificial Intelligence algorithms may become more adaptive to novel circumstances, and may not need mathematical models when data is enough [37]. Staszak [38] highlighted AI-based chemical kinetics modelling advances, which are vital to industrial reactor design and analysis. It tests AI-driven reaction kinetics prediction methodologies, notably neural network and training methods, across multiple chemical processes. Taheri et al [39] investigated the use of artificial intelligence (AI) approaches in forecasting transmembrane pressure (TMP), a critical operational parameter in anaerobic membrane bioreactor-sequencing batch reactor (AnMBR-SBR) systems used for biohydrogen generation. Using input parameters including organic loading rate (OLR), effluent pH, mixed liquor suspended solids (MLSS), and mixed liquor volatile suspended solids (MLVHS), the study contrasts two AI-based models: artificial neural networks (ANNs) and adaptive neuro-fuzzy inference systems (ANFIS). Particularly using the Gauss membership function, the ANFIS model—trained using hybrid algorithms—achieves exceptional prediction accuracy. These results show how well artificial intelligence-driven modelling may improve process control and efficiency in biohydrogen generation and wastewater treatment. Zhang et al [40] studied an AI-assisted design strategy to optimise the continuous oxidation of 2-ethylhexanol (2-EHA) into 2-ethylhexanoic acid (2-EHAD), addressing the inefficiencies and excessive energy consumption of batch procedures An accurate reactor surrogate model accelerates reactor internal optimisation, boosting the relevance of sparse experimental data owing to extended operation cycles and oxygen safety issues. This technology increases economic profit by 30–40% and reduces carbon emissions by 10–50% compared to batch and butyraldehyde-based methods. This technique improves continuous oxidation process design, improving industrial chemical production efficiency and sustainability .Artificial intelligence involves simulating human cognition in computers designed to model human thinking and behavior [41]. The optimal function of Artificial Intelligence is its ability to analyze and execute actions that are most likely to achieve a particular goal. Artificial Intelligence encompasses a range of techniques and methods applicable to optimization and modeling [42] its improves the ability to analyze past data in order to predict future patterns and behaviors [43]. Over the past several decades, various types of Artificial Intelligence modeling methodologies such as neural networks (NNs), expert systems, fuzzy logic, and Gaussian processes have been used for data classification, fault detection and diagnosis, chemical process design, and monitoring and control [44]. The chemical processing industry has relied on modeling techniques to monitor, control, optimize, and design processes, especially since the Third Industrial Revolution and the emergence of process systems engineering [45].

3.1 Machine learning

Machine learning, an application of artificial intelligence, data can be text, images, or anything else that is stored digitally. The process of using algorithms to interpret data, learn from it, and then make predictions about unseen data without being explicitly programmed to do so,uses statistical approaches to discover patterns in data [[46], [21]]. Machine learning can capture the dynamics of complex and nonlinear chemical processes from operational data [47]. It is generally classified into three categories: supervised learning, unsupervised learning, and reinforcement learning [48] [49]. It has provided an alternative to traditional control methods. Recently, deep reinforcement learning (DRL) has emerged as a prominent subfield within the machine learning community due to its excellent effectiveness in control tasks [50]. Machine learning techniques have been used to model chemical processes using data in situations where first-principle models are not available [[51],[52]]. Mowbray et al [53] monitored batch process quality using real-time process data and powerful machine learning to take advantage of the Fourth Industrial Revolution. Integrating latent variable models with probabilistic machine learning to create soft sensors improves traditional monitoring approaches. These sensors estimate prediction uncertainty and capture process data nonlinearities to enhance predictions. The suggested technique improves industrial batch process quality monitoring, notably in forecasting non-Newtonian fluid final viscosity, making batch operations more efficient and dependable. Mehrani et al [54] introduced a new method for estimating N_2O emissions in wastewater treatment facilities (WWTPs) using mechanistic modelling and ML algorithms. A mechanistic model simulated two 15-day experiments in a nitrifying sequencing batch reactor, yielding input data such NH_4-N, NO_2-N, NO_3-N, MLSS, MLVSS, and online measurements (DO, pH, temperature). Three ML models: ANNs, GBMs, and SVMs were trained and evaluated, with ANNs having the highest predicted accuracy. Validated using 95% confidence interval analysis, the ANN model is reliable for N_2O emission forecasting, optimising WWTP operations and lowering greenhouse gas emissions.[55] optimises batch crystallisation processes utilising machine learning-based predictive control, focussing on seeded fesoterodine fumarate cooling crystallisation and dissolution. Due of insufficient experimental data, the study builds a one-dimensional population balance model utilising empirical kinetic parameters to predict crystal nucleation, growth, and agglomeration .

3.2 Artificial neural networks

They are computational models used to model data, based on their name, which reflects their basis in the organic nervous system. Artificial neural networks (ANNs) use a multi-layered architecture that mimics the human brain [56]. Neurons as shown in Figure (1) are interconnected components and processing elements found in ANNs [57]. These neural configurations address many challenging challenges by working in unison. Large amounts of data with complex properties can be studied using neural networks. Furthermore, neural networks are valuable for many industrial uses, enabling prediction of certain behaviors, identifying anomalies or errors in data, etc. Because their inputs are stored within their own networks, neural networks are an excellent tool for processing complex nonlinear communications [[19],[58],[59],[34]]. Many types of neural networks use distinct concepts to create rules for different applications and form the basis for most pre-trained models. Three particularly well-known neural networks are artificial neural networks (ANNs), convolutional neural networks (CNNs), and regression neural networks (RNNs) [21]. Artificial neural networks have been mostly used in process engineering for process modeling, process control, fault diagnosis, fault identification, data standardization, and process analysis so far [[60],[61]]. Sadeghzadeh et al [62] optimised the Fenton method for decolorising industrial wastewater by removing Direct Red 16 (DR16) dye utilising a heterogeneous Fenton reaction in a microchannel reactor. Experimental data was used to create an ANN model to predict and optimise decolorisation efficiency. The model's predictive power was confirmed by experiments. The ideal operating parameters were determined using a genetic algorithm (GA), which showed that greater dye concentrations (10–40 mg/L) increased decolorisation efficiency. Ammar et al [60] used artificial neural networks (ANNs) to quickly generate prediction models from experimental batch process data. The approach estimates chemical species concentration evolution as a function of operational parameters using recurrent neural networks (RNNs). A global ANN-based model is created from these models for reliable time-series predictions. The esterification of methanol by acetic acid validates the approach's ability to capture kinetic behaviour under different circumstances. Adding the global ANN model to a hybrid modelling framework allows the process to be expanded to a semi-batch chemical reactor. This research shows how data-driven modelling may improve chemical engineering process knowledge and scalability.

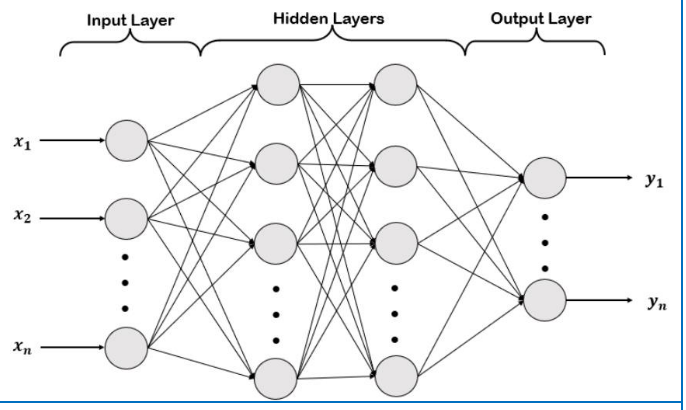

Fig. 1 Architecture of an artificial neural network. [63]

3.3 Genetic algroithms

Genetic Algorithm (GA) is a heuristic search method that operates on a population of potential solutions, analogous to the biological processes of population genetics and natural selection. It employs a recursive method to get the optimal answer via several alternatives. In genetic algorithms, all potential solutions are represented as genes composed of character strings derived from certain alphabets. New solutions are produced by mutation among the current population members, and ultimately, two solutions are amalgamated through mating to create a new solution[36]. As shown in figure(2). Genetic algorithms (GAs) are a kind of optimisation tool that draws on research in natural genetics and natural selection. The basic idea behind it is that the strongest members of a population have the highest chance of surviving. Genetic algorithms provide a holistic perspective grounded on biological analogies. Several features set the genetic algorithm apart from competing optimisation methods: The genetic algorithm uses coded representations to make decisions rather than directly modifying the variables ,the evolutionary algorithm searches across a pool of possible solution points rather than focussing on a single ideal point, the goal function is the only source of data used by the genetic algorithm. Genetic algorithms use probability transition rules instead of deterministic laws [64]. An evolutionary algorithm (GA) is a stochastic optimisation approach that is inspired by natural evolution. It is one of the metaheuristic algorithms that is used the most often . There are evolutionary concepts that are included into a GA process. These principles include chromosomal mutations and crossover. The target issue is expressed in the form of a binary string, and each chromosome acts as if it were its own particular solution to the problem. The initial population of chromosomes is formed in a random fashion, and for reproduction purposes, the chromosome that provides a more satisfactory answer to a predetermined objective is selected . The whole process of optimisation may be broken down into six distinct stages: initialisation, fitness calculation, termination by a condition check, selection, crossover, and mutation. As shown in Figure 2, the process of a GA is shown in further detail. During the process of determining fitness, only the chromosomes that have shown an outstanding performance are kept for the purpose of subsequent reproduction. In order to significantly increase the likelihood of acquiring better chromosomes, this process of selection and reproduction is repeated several times. The following phase involves the superior chromosomes producing kids via the process of crossover, which involves the exchange of string sections and gene combinations. This results in a new solution. During the process of mutation, one of the chromosomes is chosen to undergo arbitrary swapping in order to modify a predetermined bit that has been chosen at random. In order to determine whether or not the created solution is suitable, it is evaluated and compared to the termination criteria. When all of the termination conditions have been met, the GA process will come to an end [[65], [66]] . The genetic algorithm is a well recognised optimisation technique. Initially, the algorithm generates a population of μ random possible solutions (the individuals). Subsequently, in each iteration, the reproduction operator randomly generates a temporary population of λ individuals. Members of this population receive modification by crossover and mutation operators, facilitating both exploitation and exploration of the solution space. Subsequently, the μ optimal people (in terms of the objective function) are transferred to the subsequent iteration [51].

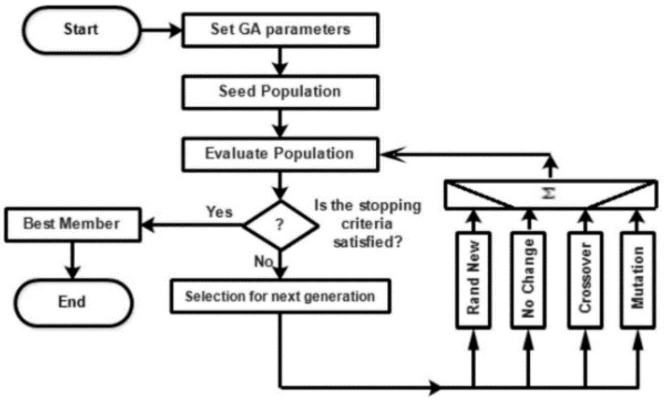

Fig. 2 Genetic algorithm process flowchart.[67]

Technique	Main Applications	Advantages	Disadvantages
Machine Learning	- Modeling nonlinear chemical processes where first principle models are unavailable [52] - Fault detection and process monitoring [53] - Predictive control [54]	- Capable of learning complex data patterns [47] - Suitable for real-time control [50]	-Requires large datasets and limits interpretability [52]
Artificial Neural Networks (ANNs)	-Time-series modeling and nonlinear data analysis [60] - Fault diagnosis and detection [19] - Process optimization in chemical engineering [62]	- High prediction accuracy [58] - Handles complex nonlinear data [61] - Supports various types like CNN and RNN [21]	- Risk of overfitting [61] - Difficult to interpret results [19]
Genetic Algorithms (GA)	-Optimization of process parameters [36] - Training neural network weights [68].	- Global search capability avoiding local minima [64] - Does not rely on gradient information	- Computationally intensive and Slow convergence in some problems [65].

	- Metaheuristic optimization inspired by natural selection [65].	[51].	

Table1: Comparison of Artificial Intelligence Techniques Used in Batch Reactor Processes.

3 . Hybrid modeling approach

4.1 A genetic algorithm and a neural network (GA-ANN)

There are three main steps to using an ANN together with a genetic algorithm for weight training. The first step is to choose a way to represent the connection weights; for example, you may use a binary connects form or just use actual numbers.Step two involves building the appropriate neural network and evaluating the fitness of these link weights. The third one involves using a genetic algorithm to apply the evolutionary process in a fitness-based manner, which includes operations like mutation, selection, and crossover. If the fitness is less than a certain threshold, evolution will halt. There are two parts to the hybrid network learning process. The first part involves using GA to find the best or almost best connection weights and thresholds for the network. Afterwards, the final weights will be adjusted using the ANN. Using a GA-ANN hybrid allows one to discover the best possible value for network weights. Following the initialization of the population, the total mean square error is used to measure the fitness of each chromosome. Once all chromosomes have been evaluated, the repro-duction operator is used to take chromosomes from the present population in order to produce an intermediate population. Lastly, the chromosomes of the intermediate population are subjected to the crossover and mutation operator in order to generate the population of the following generation. Following the reproduction of new chromosomes by selection, crossover, and mutation operators, they are assessed. This procedure is repeated for all chromosomes until a stopping threshold is met. The core principle of genetic algorithms (GA) is that, via the process of natural selection, populations may be enhanced in terms of fitness as individuals are handed down through generations. A member of the fitness population with the highest starting point is used to initialize the artificial neural network (ANN) weights and thresholds [68].

4.2 Adaptive Neuro-Fuzzy Inference system (ANFIS)

Traditional modeling methods struggle with nonlinear and dynamic problems, to address this, Jang (1991) developed a fuzzy inference system. He integrated it with neural networks to overcome the limitations of conventional approaches [85]. First, theory was used to create the Adaptive Neuro-Fuzzy Inference System (ANFIS). There is a neural network theory, a fuzzy system for thinking, and a generalized neural network. The fuzzy system is a layered feed-forward neural network made up of nodes and neurons that connect the input to the output through different layers. The second theory is called the Fuzzy Inference System. It is mostly made up of if-then rules, and each fuzzy rule describes how a network acts locally. The ANFIS model was made up of 5 layers. Layer 1 was the input layer, Layer 2 was the firing strength of a rule, Layer 3 was a list of all the firing strength rules, Layer 4 was the consequent layer, and Layer 5 would figure the total and give the out put that was needed. ANFIS is used in many areas where working with a lot of nonlinearity is necessary. To keep the settings up to date, ANFIS uses a special algorithm called a hybrid-learning algorithm. This algorithm is made up of two parts: the gradient descent method and the least-squares method. There are five layers, and each of these algorithms works on a different one.

The gradient descent method tunes the nonlinear parameters in layer 1, while the least-square method tunes the parameters in layer 4 [42].

Hybrid Technique	**Main Applications**	**Advantages**	**Advantages**
GA-ANN (Genetic Algorithm with Artificial Neural Network)	-Optimizing connection weights in neural networks - Training ANN when local minima or slow convergence are issues - Used for modeling and control of batch processes [68].	-Combines global search capability of GA with fine-tuning accuracy of ANN, leading to better convergence and avoiding local minima [68]. - Effective in modeling complex nonlinear systems with improved learning stability [65]	- High computational cost due to iterative evolutionary operations - Requires careful parameter tuning; increased system complexity[66]
ANFIS (Adaptive Neuro-Fuzzy Inference System)	- Control and modeling of highly nonlinear, time-varying systems [42]	- Integrates human-explainable fuzzy logic with learning capability of ANN and Hybrid learning (gradient descent + least squares) enables fast and accurate rule adjustment [42]	-Training is [69]computationally expensive and may require large, high-quality datasets [21] - Rule explosion can occur with many inputs, reducing scalability [58]

Table 2: Comparison of Hybrid Artificial Intelligence Techniques.

5 . Applications of **Artificial Intelligence** *in Batch Processes.*

5.1 Optimization of adsorption water treatment process

The biggest problem of our time is getting clean water to drink. This is also one of the main goals of the UN's sustainable development goals (SDGs) . On the other hand, river pollution from fast population and industrialisation growth has become a major environmental problem in the last few years .Artificial intelligence (AI) has become a strong tool for solving problems in the real world. It has gotten a lot of attention because it can be used in so many areas. In the past few years, AI has also been used in water treatment and electrolysis to make the process more efficient and to find real-world answers to problems like water pollution and lack of water. [69]used AI-based models to improve membrane bioreactors (MBRs) for sustainable wastewater treatment. Machine learning and neural networks predicted optimal operational parameters like water flow rate, temperature, and pollutant concentration. AI integration increased treatment efficiency by 18% and reduced energy consumption by 12% compared to conventional methods. [70] predicted TMP in an AnMBR-SBR reactor using ANN and ANFIS. The ANFIS model had a high predictive accuracy of $R^2 = 0.93$ ($MSE = 7.3 \times 10^{-3}$), while the ANN model had $R^2 = 0.88$. These predictive models improved membrane fouling control, increasing reactor efficiency by 14%. [36] found that AI-optimized chemical dosing and real-time monitoring can cut water treatment plant operational costs by 20–30%. Machine learning models can also detect water quality changes early, predict contaminant transport, and improve system performance beyond human operation. However, artificial intelligence (AI) has shown that it has the potential to solve problems in drinking water treatment (DWT). This is because AI can learn on its own and solve difficult issues. AI technology helps handle and run DWT processes technically, which is more efficient than depending only on people to do the work. AI-based data analysis and genetic learning systems can diagnose water quality, make decisions on their own, and improve operation processes. They could also be used to create a platform for all process analysis and predictive modeling. AI technologies, not like mathematical models or statistical methods, are very good at dealing with complicated nonlinear relationships and having a good grasp of how water treatment systems work as a whole. So, AI technologies can track how water quality changes over time, analyze and predict water quality, and show how pollutants move and change form. This means that the focus can shift from fixing problems that are already happening to finding risks ahead of time and making facilities work better all the time [71].

5.2 *Optimization of* Pharmaceutical Batch *process.*

Artificial intelligence has emerged as a transformative force in the fields of pharmaceutical technology and drug delivery design. By analyzing genomics and proteomics data, AI algorithms are able to predict drug interactions and identify disease-associated targets, thereby increasing the probability of successful drug approvals and reducing costs by optimizing RD&D processes. In 2023, [72]. reported that machine learning models were able to predict pharmacokinetic properties, including absorption and stability, with an accuracy of up to 85%. Additionally, they were able to reduce the number of experimental batches by 30%. AI-driven systems also improved the performance of microneedle arrays for long-acting drug delivery by decreasing manufacturing variability by 18% and increasing release reliability by 25%. Additionally, nanocarrier design models for ocular drugs exhibited a 90% predictive accuracy, resulting in a 1.5-fold increase in bioavailability. These discoveries suggest that AI not only expedites drug discovery and formulation but also enhances the efficacy of dosage forms and decreases development costs and time. Consequently, it presents promising opportunities for the advancement of pharmaceutical research and development in the future.

5.3 Fermentation Process Control and Optimization

It is essential to have process management and optimisation in place in order to guarantee that a process will continue to provide a profitable revenue while also preserving the needed level of quality. In comparison to the standard chemical method, the fermentation process has a lesser effect on the environment and much cheaper operating costs, both of which have contributed to its growing popularity [63]. [73] developed a hybrid modelling technique for large-scale fermentation processes (above 100,000 gallons) to solve the constraints of classic kinetic models with insufficient system information. Researchers use kinetic and data-based models to improve accuracy and robustness using data-driven modelling. The work refines the kinetic model using process information, This method enhanced prediction accuracy by up to 20% relative to traditional models and was validated using industrial-scale data, indicating improved robustness and reliability for process optimization. The hybrid method is promise for optimising industrial bioprocesses due to its accuracy and versatility Fermentation processes are prevalent in the manufacture of many industrial chemicals, bulk enzymes, food items, and medicines . Improvements in productivity have been achieved by the creation of resilient industrial host strains. Upon obtaining a developed strain, the objective is to devise a fermentation procedure that establishes the best circumstances for the specific strain during the fermentation period. Batch fermentations are the simplest to manage, since all carbon sources and media components are supplied simultaneously at the commencement of the fermentation, which continues until the carbon source is exhausted. This is easy to run; yet, it necessitates extended downtime for batch processing. It is also inefficient due to fluctuating substrate concentrations and does not permit regulation of growth rates or product creation rates. The issue lies not only in sustaining the ideal feed rate but also in determining how the optimal feed rate is defined. This is a multifaceted problem dependent upon the procedure and output. Model predictive control is a prevalent control methodology owing to its capacity to manage complex multivariate systems. Originating from the petrochemical sector, Industrial studies indicate that the implementation of MPC can enhance fermentation productivity by 10-25%, decrease substrate consumption by as much as 15%, and reduce downtime between batches by 30% through optimized feeding strategies and real-time trajectory adjustments. Endpoint MPC, implemented upon batch completion, guarantees product quality through continuous monitoring and adjustment of the process trajectory. The selection of optimization objective functions and constraints is contingent upon particular industrial needs.[15].

6. Challenges and Limitations

There are numerous obstacles associated with batch processing. There is a necessity for enhanced data-driven control and optimisation methods, as there is limited time to develop suitable dynamic models. These methods necessitate the availability of online specific measurements, which are not yet routinely available in production. The primary operational challenge in batch-process optimisation is the prevalence of run-end outputs, such as final quality, which are not measurable during the run. This is a technical issue. Process models in the batch domain are generally subpar, despite the availability of model-based solutions. Conversely, the challenge of measurement-based optimisation for a specific batch is that it necessitates knowledge of the future in order to make decisions during the batch. Consequently, the primary focus of the research is on the utilisation of data from both the current and previous cohorts for the purpose of control and optimisation, as well as measurement-based optimisation [9] . A significant obstacle that this new shift must overcome is the fact that AI algorithms need a significant amount of computer resources. Because of this reality, there is a drive to improve hardware acceleration in order to provide the necessary high computing power. Demand for high-performance compute resources is one of the primary obstacles that is preventing artificial intelligence from reaching its full potential [74] . While AI presents numerous advantages, there exist certain limitations that impede the broader implementation of these techniques in practical scenarios. The accessibility and variety of data, along with inadequate reproducibility, The computational demands are substantial, and the interpretation of the trained models poses significant challenges[36]. The "generalisation gap" is another issue that arises in relation to big batch training, as Keskar et al. (2016) came to find. They ultimately came to the conclusion that "the lack of generalisation ability is due to the fact that large-batch methods tend to converge to sharp minimizers of the training function." A number of approaches, including data augmentation and warm-starting with tiny batches, were attempted by them in an effort to enhance the generalisation; nevertheless, they were unable to identify a solution that was successful [75] . There is still a limited amount of actual use of this kind of advanced control in the industrial sector. As a result of the complexity of advanced controller design, extra installation costs are required for costly measurement equipment, and there is a dependency on the quality and accuracy of the process model, particularly for model-based controllers [63] . Even though this growth has been life-changing, there are still problems and issues that need to be addressed. AI systems don't always have their own problems. For example, they need to make sure that the data is correct, that it is valid from outside sources, and that it is safe [49]. Though they offer some advantages, AI-based models have certain drawbacks like the need for big datasets, possible prejudices, and lack of interpretability. Therefore, to guarantee the safety and efficiency, artificial intelligence-based models should be used in cooperation with conventional experimental techniques [72] .One the one hand, AI and ML algorithms often place heavy demands on computer resources. For instance, in order to speed up the training process on large data [49], but existing manufacturing facilities do not have the processing power to meet such demanding standards. Consequently, it is usual practice to entrust the processing of industrial data to third-party cloud computing service providers. Nevertheless, there is a chance that sensitive information (such as individualised product designs) or private consumer data may be leaked if the production data is outsourced to a third party. Conversely, time-sensitive activities cannot be met in real-time due to the substantial latency that results from transmitting manufacturing data to distant clouds[76]. The level of complexity of advanced control systems is always increasing. Reliability, acceptable performance, and environmental protection are particularly important for safety-critical systems, such chemical processes. Severe financial, human, and environmental consequences may result from an error. Therefore, problem detection and live monitoring are becoming more important for enhancing system dependability. Thus, it is possible to implement the early warning signals and avert the system's shutdown and, to a considerable degree, a disaster [77].

7. Future Trends and Research Directions

A promising new technology that promises to solve modern plants' problems in novel ways is cyber physical systems (CPS), which integrate and deeply collaborate with 3C (Computer, Communication, Control) technologies to realise the organic of large-scale engineering systems' real-time perception, dynamic control, and information services. The five capabilities of computing, communication, precise control, remote coordination, and autonomy are made possible by connecting the physical device to the internet via CPS. One of the pioneering approaches to plant process automation among these CPS technologies is economic model predictive control (MPC), a control system for industrial processes that uses optimisation economics as an indicator [78]. These are only a few of the many potential directions for future research. By adding a safe reinforcement learning algorithm that guarantees adequate performance and/or respects safety requirements during training, you may create safe online adaption techniques.Conduct a methodical examination and formulate a set of recommendations for the incentive structure that is most appropriate for accomplishing certain control goals, such as tracking, constraint fulfilment, and economic optimisation and Create an automated process for figuring out RL hyperparameters [1].
Despite significant advancements, many potential research opportunities exist. These involve:

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Despite significant advancements, several key research directions remain open in the application of AI to batch chemical processes:

1. Improving Model Accuracy and Robustness:
   One major challenge is building dynamic models that accurately capture the nonlinear, time-varying behavior of batch reactors, especially under disturbances or varying operating conditions. Future work should focus on hybrid models that combine first-principles with AI-based learning, which can improve predictive accuracy while retaining interpretability.

2. Real-Time Optimization and Control under Uncertainty:
   Batch processes often face variability in feed composition, temperature, and reaction kinetics. Developing real-time optimization frameworks—particularly those based on **Model Predictive Control (MPC)** enhanced with AI—is a promising path. For example, integrating reinforcement learning with MPC could enable adaptive control policies that self-improve through real-time feedback.
3. Data-Driven Control Systems:
   There is growing potential in leveraging large datasets from industrial operations to construct purely data-driven models using deep learning or ensemble techniques. These models can then be used in control systems without the need for complete mechanistic understanding, especially in systems where reaction mechanisms are unknown or highly complex.

Recommendations:
To advance industrial adoption, future research should focus on developing AI-based digital twins, building adaptive control systems with online learning capabilities, and creating AI platforms that integrate seamlessly with existing industrial control infrastructure. Such advancements can reduce energy consumption, increase product yield, and improve safety in chemical manufacturing.

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8. Conclusion

The dynamic modelling and control of batch reactors present significant challenges in chemical engineering due to their intrinsic nonlinearity, time-varying characteristics, and inadequate process comprehension. Artificial Intelligence (AI) methodologies—such as machine learning, deep learning, and hybrid models—exhibit significant potential in addressing these constraints by facilitating data-driven insights, accurate predictions, and adaptive control strategies. These methodologies improve process efficiency, product quality, and safety, particularly in situations where first-principles models are inadequate or impractical. AI methodologies possess the capability to identify concealed patterns, adjust to variable operational conditions, and facilitate real-time decision-making, rendering them especially appropriate for the dynamic characteristics of batch processes. Hybrid AI models that integrate data-driven learning with physical comprehension effectively reconcile interpretability and performance. Nonetheless, numerous practical obstacles persist, such as the necessity for high-quality data, integration with current industrial control systems, computational expenses, and a deficiency of transparency in black-box models. These constraints highlight the necessity for additional research concentrated on explainable AI, transfer learning in low-data contexts, and scalable frameworks compatible with industrial systems. Future research should focus on the standardisation, validation, and generalisation of AI models across various chemical systems. The creation of benchmark datasets and open-access modelling tools can enhance reproducibility and collaboration. The incorporation of AI into batch reactor modelling and control signifies a transformative change that could redefine process optimisation, sustainability, and automation within the chemical sector.

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