Mohsen Pirdashti, Silvia Curteanu*, Mehrdad Hashemi Kamangar, Mimi H. Hassim and Mohammad Amin Khatami

Artificial neural networks: applications in chemical engineering

Abstract: Artificial neural networks (ANN) provide a range of powerful new techniques for solving problems in sensor data analysis, fault detection, process identification, and control and have been used in a diverse range of chemical engineering applications. This paper aims to provide a comprehensive review of various ANN applications within the field of chemical engineering (CE). It deals with the significant aspects of ANN (architecture, methods of developing and training, and modeling strategies) in correlation with various types of applications. A systematic classification scheme is also presented, which uncovers, classifies, and interprets the existing works related to the ANN methodologies and applications within the CE domain. Based on this scheme, 717 scholarly papers from 169 journals are categorized into specific application areas and general (other) applications, including the following topics: petrochemicals, oil and gas industry, biotechnology, cellular industry, environment, health and safety, fuel and energy, mineral industry, nanotechnology, pharmaceutical industry, and polymer industry. It is hoped that this paper will serve as a comprehensive state-of-the-art reference for chemical engineers besides highlighting the potential applications of ANN in CE-related problems and consequently enhancing the future ANN research in CE field.

Keywords: artificial neural networks; chemical engineering applications; modeling; optimization.

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1 Introduction

In 1888, Lewis Mills Norton, a professor at the Massachusetts Institute of Technology, created a specialized program within the Chemistry Department, which blended mechanical engineering and applied chemistry, with the goal to focus on industrial practice. It is called chemical engineering (CE). CE is one of the main driving forces in promoting the development of process and technology innovation in all areas. It is a vital discipline of diverse industries including petrochemicals, oil and gas industries, manufacturing, pharmaceuticals, health care, design and construction, pulp and paper, food processing, specialty chemicals, polymers, biotechnology, nanotechnology, and environmental protection (Villermaux 1993, Favre et al. 2002, 2008, Perkins 2003, Cecchi 2007, Churchill 2007).

Traditional approaches for solving CE problems usually have limitations because of highly complex and nonlinear systems. Different techniques have been proposed for such types of processes (Shacham and Brauner 2008, Precup et al. 2009, Cole et al. 2012), but artificial neural networks (ANN) are recommended computational tools mainly because they do not require the knowledge of physical and chemical laws that govern the processes. In addition, once developed and trained, an ANN is able to make predictions in a facile manner, which is useful for chemical engineers.

The original work on neural networks (perceptrons, as they were called at that time) was published nearly 70 years ago by McCulloch and Pitts (1943, 1947) and Hebb (1949). However, since the late 1980s, there has been a dramatic growth in the level of research activity in ANNs, accompanied by an extensive coverage in the popular press (Bishop 1994, Yang and Wei 2006). ANNs have been applied to CE over many years (the 100th centenary of that program, approximately) and the first effort was done by Hoskins and Himmelblau (1988), who applied ANNs to error diagnosis for a chemical process. Since then, ANNs have been widely used for various applications in the CE field.

During the past decades, a large number of reviews have been conducted concerning the application of ANNs in CE. Hussain (1999) summarized the applications of

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Advanced Applications for Artificial Neural Networks Adel El-Shahat,2018-02-28 In this book highly qualified multidisciplinary scientists grasp their recent researches motivated by the importance of artificial neural networks It addresses advanced applications and innovative case studies for the next generation optical networks based on modulation recognition using artificial neural networks hardware ANN for gait generation of multi legged robots production of high resolution soil property ANN maps ANN and dynamic factor models to combine forecasts ANN parameter recognition of engineering constants in Civil Engineering ANN electricity consumption and generation forecasting ANN for advanced process control ANN breast cancer detection ANN applications in biofuels ANN modeling for manufacturing process optimization spectral interference correction using a large size spectrometer and ANN based deep learning solar radiation ANN prediction using NARX model and ANN data assimilation for an atmospheric general circulation model Modeling and Simulation in Chemical Engineering Christo Boyadjiev,2021-12-08 This book presents a theoretical analysis of the modern methods used for modeling various chemical engineering processes Currently the two primary problems in the chemical industry are the optimal design of new devices and the optimal control of active processes Both of these problems are often solved by developing new methods of modeling These methods for modeling specific processes may be different but in all cases they bring the mathematical description closer to the real processes by using appropriate experimental data In this book the authors detail a new approach for the modeling of chemical processes in column apparatuses Further they describe the types of neural networks that have been shown to be effective in solving important chemical engineering problems Readers are also presented with mathematical models of integrated bioethanol supply chains IBSC that achieve improved economic and environmental sustainability The integration of energy and mass processes is one of the most powerful tools for creating sustainable and energy efficient production systems This book defines the main approaches for the thermal integration of periodic processes direct and indirect and the recent integration of small scale solar thermal dryers with phase change materials as energy accumulators An exciting overview of new approaches for the modeling of chemical engineering processes this book serves as a guide for the important innovations being made in theoretical chemical engineering *Application of Artificial Intelligence in Wastewater Treatment* Shikha Gulati,2024-09-09 This book offers a comprehensive exploration of the integration of artificial intelligence AI techniques in addressing challenges and optimizing processes within wastewater treatment The coverage of the book spans a spectrum of applications including AI driven monitoring and control systems predictive modeling for pollutant removal and the development of smart sensor networks for real time data analysis in wastewater treatment plants By amalgamating AI methodologies with wastewater treatment processes the book provides insights into enhancing efficiency reducing costs and mitigating environmental impacts In the current research scenario the theme of the book is highly pertinent as it responds to the pressing need for sustainable and

efficient wastewater treatment solutions The book defines the theme by elucidating how AI technologies such as machine learning algorithms and data analytics can revolutionize wastewater treatment processes by enabling proactive decision making optimizing resource allocation and predicting potential system failures This intersection of AI and wastewater treatment not only addresses operational challenges but also contributes to the broader goal of achieving environmentally conscious and economically viable solutions **Elements of Artificial Neural Networks with Selected Applications in Chemical Engineering, and Chemical and Biological Sciences** Sanjeev S. Tambe,Bhaskar D. Kulkarni,Pradeep B. Deshpande,1996 Machine Learning Tools for Chemical Engineering Francisco Javier López-Flores,Rogelio Ochoa-Barragán,Alma Yunuen Raya-Tapia,César Ramírez-Márquez,José Maria Ponce-Ortega,2025-05-15 Machine Learning Tools for Chemical Engineering Methodologies and Applications examines how machine learning ML techniques are applied in the field offering precise fast and flexible solutions to address specific challenges ML techniques and methodologies offer significant advantages such as accuracy speed of execution and flexibility over traditional modeling and optimization techniques This book integrates ML techniques to solve problems inherent to chemical engineering providing practical tools and a theoretical framework combining knowledge modeling representation and management tailored to the chemical engineering field It provides a precedent for applied Al but one that goes beyond purely data centric ML It is firmly grounded in the philosophies of knowledge modeling knowledge representation search and inference and knowledge extraction and management Aimed at graduate students researchers educators and industry professionals this book is an essential resource for those seeking to implement ML in chemical processes aiming to foster optimization and innovation in the sector Outlines the current and potential future contribution of machine learning the use of data science and ultimately how to correctly use machine learning tools specifically in chemical engineering Devoted to the correct application and interpretation of the results in various phases of the development of decision support systems data collection model development training and testing as well as application in chemical engineering Examines chemical engineering specific challenges and problems including noise manufacturing equipment and domain specific solutions such as physical knowledge using relevant case study examples **Deep Learning Applications** Pier Luigi Mazzeo,Paolo Spagnolo,2021-07-14 Deep learning is a branch of machine learning similar to artificial intelligence The applications of deep learning vary from medical imaging to industrial quality checking sports and precision agriculture This book is divided into two sections The first section covers deep learning architectures and the second section describes the state of the art of applications based on deep learning Artificial Neural Networks in Chemical Engineering Processes Ahad Ghaemi,Zohreh Khoshraftar,2026-02-01 Artificial Neural Networks in Chemical Engineering Processes From Theory to Applications serves as a comprehensive resource on artificial neural networks within chemical engineering including understanding the fundamental principles learning about relevant algorithms and architectures and exploring practical case studies This book covers theoretical principles relevant algorithms

and practical case studies this book covers artificial neural network concepts architectures and algorithms with a focus on applications in chemical engineering processes This book also addressed common challenges by providing practical guidance through successful case studies offering insights on data pre processing model selection training strategies and performance evaluation The book serves as a valuable tool for bridging the gap between neural networks and their practical implementation in chemical engineering This book will be an invaluable resource for chemical Engineers particularly researchers and industry professionals working in Machine Learning and Artificial Intelligence It will also be a very useful guide for Graduate and Postgraduate Students in Chemical Engineering and machine learning Artificial Neural Networks in Chemical Engineering will also be a valuable resource for anyone working with artificial neural networks in other industries particularly data scientists and analysts Serves as a comprehensive resource to bridge the gap between theoretical knowledge of neural networks and practical implementation in chemical engineering In depth explanations of neural network concepts architectures and algorithms with specifics about applications in chemical engineering Outlines various types of artificial neural networks including feed forward networks and their applications in chemical engineering processes and systems Practical guidance and case studies showcasing the successful application of neural networks in solving chemical engineering problems Insights into essential aspects such as data pre processing techniques model selection training strategies and performance evaluation to provide a roadmap for the effective implementation of neural networks in experimental modelling including code and MATLAB modelling   *Biotechnological Applications of Biomass* Thalita Peixoto Basso,Thiago Olitta Basso,Luiz Carlos Basso,2021-08-18 Biotechnological Applications of Biomass provides a comprehensive overview of the current state of the art of biomass utilization in agriculture and pharmaceuticals The information contained herein is useful to researchers and other readers interested in biomass utilization and production of bioproducts

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know the frontiers of the control technology *14th International Symposium on Industrial Crystallization* ,1999 This conference provides a forum for discussion of the advances in the theory and practice of crystallization as it relates to the production of bulk crystalline materials *Artificial Intelligence for Chemical Sciences* Shrikaant Kulkarni,Shashikant Bhandari,Dushyant Varshney,P. William,2025-05-09 Chemists are increasingly employing artificial intelligence AI for diversified applications This new volume explores the use of AI and its various computer aided applications for the design of new drugs and chemical products for toxicity prediction and biodegradation and for fault diagnosis in chemical processing plants The volume explores knowledge and reasoning based approaches of the field of chemintelligence to make predictions about the right molecules with given structures and properties as precursors or starting materials reaction pathways reaction conditions improvement in reaction efficiency and selectivity toxicity metabolism biodegradation and more

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