

## Neural Networks in The Chemical Industry

Matthew N. O. Sadiku<sup>1</sup>, Sarhan M. Musa<sup>1</sup>, and Osama M. Musa<sup>2</sup>

<sup>1</sup>Roy G. Perry College of Engineering Prairie View A&M University  
Prairie View, TX 77446

<sup>2</sup>Ashland Inc, Bridgewater, NJ 08807

**ABSTRACT:** An artificial neural network (ANN) is an information processing construct inspired by the manner in which the brain processes information and were originally developed to mimic the learning process of the human brain. They have been increasingly used in the chemical industry for data analysis, process control, pattern identification, identification of drug targets, and the prediction of several physicochemical properties. This paper provides a brief introduction on neural networks and their applications to the chemical industry.

**KEY WORDS:** artificial neural networks, chemical industry, chemical engineering, modeling

### I. INTRODUCTION

Artificial neural networks (ANNs) (also called perceptron networks, connectionist systems or neurocomputers) are designed to mimic the complexities of the brain functions in an effort to capture the amazing learning capabilities of the human brain. They may be regarded as a sort of parallel processor designed to imitate the way the brain accomplishes tasks [1]. They provide a wide range of powerful new techniques for solving problems in diverse chemical engineering applications. Due to their simplicity, ANNs are a promising tool for simulating the highly interdependent variables of complex manufacturing processes. The idea of ANNs was inspired by the structure of the human brain and by an envy of what the brain can accomplish. The 1980s witnessed a resurgence of interests in ANNs. This interest was due to the development in new algorithms and VLSI. The field of neural networks and the development of neural network tools have expanded unbelievably in the past years [2]. Engineering systems are generally less complex than the brain. Various chemical processes can be described by relatively straightforward mathematical functions. Chemometrics is widely employed to solve complex chemical problems via the use of large data sets which contain embedded implicit relationships through the construction of composite, generally linear, response relationships. ANN is a non-traditional chemometric tool for providing accurate solutions to complex, non-linear problems. ANNs can be viewed as non-linear models that can represent input-output data, classify data, and recognize patterns within data. ANNs can solve practical complex tasks in a number of applications that should be of interest to chemists and chemical engineers [3]. The main advantage of ANNs is their ability to represent complex input-output relationships.

### II. CHARACTERISTICS OF ANN

An artificial neural network is an interconnection of nodes, similar to the network of neurons in a brain, working in unison to solve specific problems. The interconnections of the nodes are called synapses. ANN is a mathematical tool whose functioning is inspired by that of the human brain. Thus, an ANN basically consists of nodes (or neurons), connections (axons and dendrites) between nodes, connection weights (synapses) and thresholds. It contains an input layer, an output layer, and one or more hidden layers [4].

Different types of artificial neural networks are available: (1) support vector machine (SVM), (2) self-organization map (SOM), (3) multilayer perceptron (MLP). Typically, neurons are organized in layers. The neurons act as nonlinear processing elements within the network. Signals travel from the first (input), to the last (output) layer, possibly after traversing the layers multiple times. The number of neurons in the input and output layers are fixed based on the number of inputs and outputs. As shown in Figure 1 [5], the neurons are generally grouped into three different types of layers [6]:

- Input layer: whose number of nodes depends on input variables
- Output layer: whose number of nodes is equal to the number of predicted variables
- Hidden layer: situated between the first two layers.

Artificial neural networks acquire knowledge during a learning process and that knowledge is stored in the synaptic weights of the connections.

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## **Table of Contents Applications Of Artificial Neural Networks In Chemical Engineering**

1. Understanding the eBook Applications Of Artificial Neural Networks In Chemical Engineering
  - The Rise of Digital Reading Applications Of Artificial Neural Networks In Chemical Engineering
  - Advantages of eBooks Over Traditional Books
2. Identifying Applications Of Artificial Neural Networks In Chemical Engineering
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Applications Of Artificial Neural Networks In Chemical Engineering
  - User-Friendly Interface
4. Exploring eBook Recommendations from Applications Of Artificial Neural Networks In Chemical Engineering
  - Personalized Recommendations
  - Applications Of Artificial Neural Networks In Chemical Engineering User Reviews and Ratings
  - Applications Of Artificial Neural Networks In Chemical Engineering and Bestseller Lists
5. Accessing Applications Of Artificial Neural Networks In Chemical Engineering Free and Paid eBooks

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  - Applications Of Artificial Neural Networks In Chemical Engineering eBook Subscription Services
  - Applications Of Artificial Neural Networks In Chemical Engineering Budget-Friendly Options
6. Navigating Applications Of Artificial Neural Networks In Chemical Engineering eBook Formats
    - ePub, PDF, MOBI, and More
    - Applications Of Artificial Neural Networks In Chemical Engineering Compatibility with Devices
    - Applications Of Artificial Neural Networks In Chemical Engineering Enhanced eBook Features
  7. Enhancing Your Reading Experience
    - Adjustable Fonts and Text Sizes of Applications Of Artificial Neural Networks In Chemical Engineering
    - Highlighting and Note-Taking Applications Of Artificial Neural Networks In Chemical Engineering
    - Interactive Elements Applications Of Artificial Neural Networks In Chemical Engineering
  8. Staying Engaged with Applications Of Artificial Neural Networks In Chemical Engineering
    - Joining Online Reading Communities
    - Participating in Virtual Book Clubs
    - Following Authors and Publishers Applications Of Artificial Neural Networks In Chemical Engineering
  9. Balancing eBooks and Physical Books Applications Of Artificial Neural Networks In Chemical Engineering
    - Benefits of a Digital Library
    - Creating a Diverse Reading Collection Applications Of Artificial Neural Networks In Chemical Engineering
  10. Overcoming Reading Challenges
    - Dealing with Digital Eye Strain
    - Minimizing Distractions
    - Managing Screen Time
  11. Cultivating a Reading Routine Applications Of Artificial Neural Networks In Chemical Engineering
    - Setting Reading Goals Applications Of Artificial Neural Networks In Chemical Engineering
    - Carving Out Dedicated Reading Time
  12. Sourcing Reliable Information of Applications Of Artificial Neural Networks In Chemical Engineering
    - Fact-Checking eBook Content of Applications Of Artificial Neural Networks In Chemical Engineering
    - Distinguishing Credible Sources
  13. Promoting Lifelong Learning
    - Utilizing eBooks for Skill Development

- Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
  - Interactive and Gamified eBooks

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