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APPLIED MATHEMATICAL FIELD SUCH AS FUZZY LOGIC METHOD AND ARTIFICIAL NEURAL NETWORK WIDELY USED IN CHEMICAL ENGINEERING.

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Abstract: The purpose of this paper is to explain the application of mathematics, fuzzy logic method and artificial neural network in chemical engineering. A highly deficiency of traditional method is the fact that solving chemical engineering problems due to the majorly nonlinear behavior of chemical processes is very difficult or not possible. Today mathematical technology such as artificial intelligence (AI) techniques is becoming more useful due to easy designing, simple implementation, robustness, flexibility and generality.
The AI covers many branches, namely, artificial neural network, genetic algorithm, fuzzy logic, hybrid systems and expert systems. They have been highly used in various applications of the chemical engineering field including process control, modeling, fault detection, classification and diagnosis. In this chapter, the application of mathematic of AI is investigated in various chemical engineering fields.
Keywords: Artificial intelligent, artificial neural network, Chemical engineering, Mathematical technology.

Introduction: In the field of chemical engineering the role of mathematics is the latter half of the twentieth century. The starting of this era was taken by the concerted effort of a few to highlight the mathematical consciousness of the profession to think basically about the processes.
In the field of chemical engineering to find out the growth of the application of mathematics over the last fifty odd years. The starting of this era was marked by a shift in perspective, in which the field of chemical engineering was being taken from one that depend on a coarse terminological idea of the field into one that produce of mathematical thinking of rationality. This modification shows a drawing up to take chemical processes on a finer scale, in which organized differences contributed no more than to contrast in the details of synthesis using important unifying more elementary information. Chemical engineering had be fully grown to a field that give out with the application of scientific laws to systems, in which matter go through chemical and physical changes, with a view to control, analyze, and design them. The result of this fundamental point of view has been too much enlarging the scope of chemical engineering to give up the areas on the farther side of its original field of chemical processes. As a present, chemical engineering is a necessary component of the quantitative measurement of biomedical and biological systems, and of the combination of a various variety of materials with a magnificent range of applications. In fact, yet further appearing characteristic of originality to the profession of chemical engineering, taken in the past few years for its focus on processes, is the connected with the products design for its specific applications. But there are so many developments of technologies that have make possible the enhanced activities of the chemical trade; it could be appeared that this turn of events is also credited to the mathematical legacy that has followed the manifestation shift in the middle of the last century. This consequence is contained in the mathematical maturity of chemical engineering that is featured both in depth and breadth , and it is our objective in this article to reflect from the literature, the representation of various areas of mathematics that have been applied to chemical engineering. (This consequence of mathematical maturity of chemical engineering didn't come about without having to endure the resistance of some of the leading members of the profession at that time. Perhaps, such resistance may be viewed to have helped strengthen the foundation of the change that was occurring, but it would be well to acknowledge several activists in support such as Robert Marshall, Richard Wilhelm, Charles Wilke, , Kenneth Watson,John Davidson, Kenneth Denbigh!) Olaf Hougen, Bob Bird and Robert Pigford.

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In exploring the effect of modern mathematics on chemical engineering, it is important to discuss the steps that it engaged at some earlier period. If we talk about pre-World War II days, as they had a decided influence on the education of students in engineering and science, more in the latter than in the former. For example, electrical engineering departments in Universities prewar were primarily active in antenna theory, power, radio and control. In the previous post war era, they became active in computer design and electronics of various kinds use thus replacing more of what they had before. Prewar chemical engineering was mainly taught including excellent courses in chemistry, a few good courses stoichiometry, a survey of fluid mechanics comprising mainly hydraulics and the unit operations. On courses the remainder of the time was spent which the faculty concepts would serve the students well in the chemical industry, but, which in fact were not productive for the effort and time spent. There must have won a feeling that engineers were somehow different from other people! The mathematics offered to undergraduate students stopped with less than a full year of the calculus and with no course in ordinary differential equations. At the graduate level, the students in chemical engineering departments, where a minor was required, generally chose physical chemistry. The course load was essentially one-half that of the major, and students almost never chose mathematics or physics for their minor. Physical chemistry was generally the best choice for a minor, so that they were exposed to chemical kinetics advanced thermodynamics and statistical mechanics, which, for those students, filled an enormous void. Graduate courses offered in the chemical engineering departments were in general mimics of the undergraduate courses and were heavy with long computational problems, which were not particularly challenging, thought interesting or provoking. These courses were nonmathematical in the sense that they contained nothing beyond simple calculus.

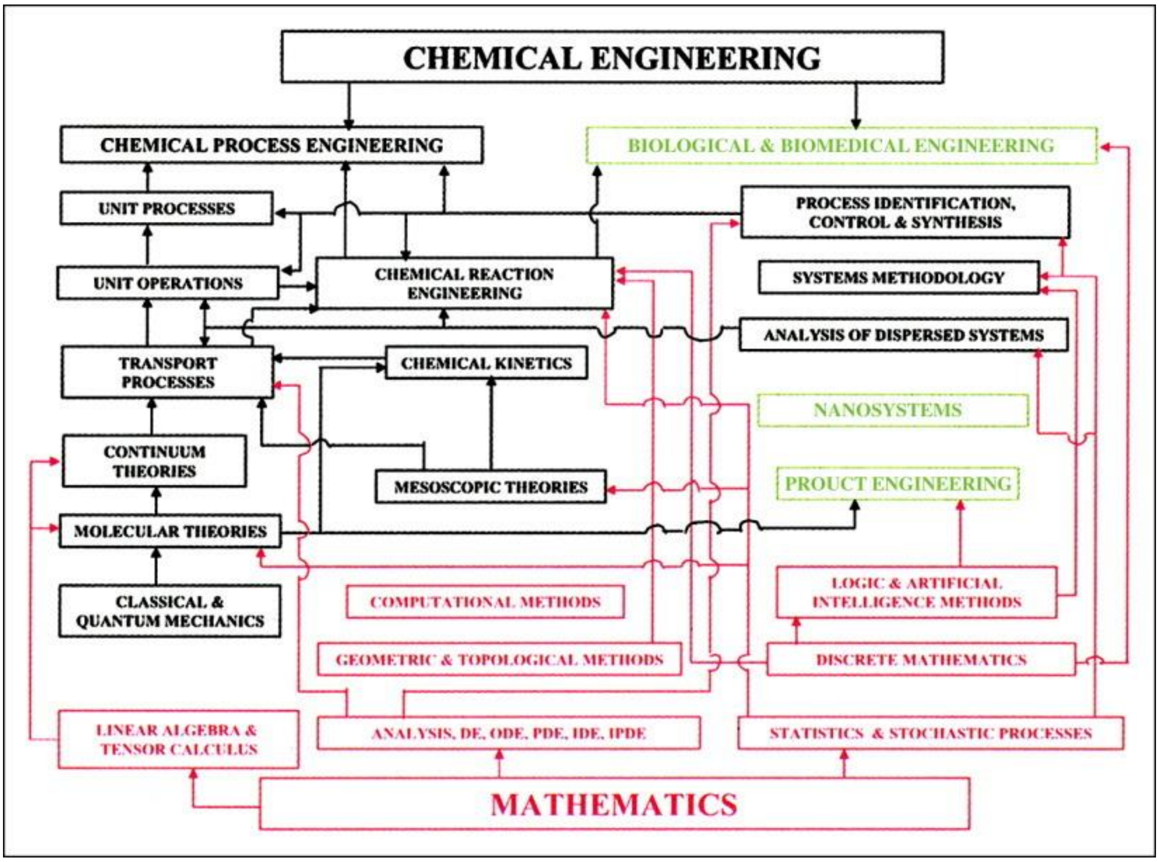

Figure 1.
Chemical engineering and mathematics.
The black color is used to represent traditional areas of chemical engineering and the green for the newer areas. Mathematics is shown in red and the arrows used to designate the areas of chemical engineering influenced by various domains of mathematics.

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Application of Artificial Neural Network in Chemical engineering

Traditional application to real chemical engineering processes modeling is depend on elementary physical and chemical laws, which include differential equations and nonlinear algebraic. From a view of computational point, these equations have some difficulties with regard to the numerical methods used for their approximation, as well as with the achievement of the desired accuracy of the calculations.

In recent years, there has been a growing interest in the application of the Artificial Neural Networks (ANNs) method to solve a number of problems in the field of chemical engineering related to fault detection, signal processing, modeling, and control of chemical and biochemical processes in which traditional modeling methods have difficulty and it is even impossible to develop physical models with acceptable errors.

Mainly, artificial neural networks are used in the following field of chemical process: physical property estimation, control, optimization of process parameters, fault diagnosis and product quality control, etc.

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. 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.

Mathematical Models for data analysis

Chemical engineers generate and use data across multiple scales - from laboratory to pilot plants to large scale industrial settings in order to construct mathematical models to understand, discover, operate, regulate or optimize the processes. However, they do not use data directly but convert it into a mathematical model, namely a set of equations that capture the essence and patterns/trends in the data as discussed below. In chemical engineering systems, there are fundamental laws that must be obeyed - these are the conservation of mass, energy and momentum. These concepts are covered in the first and second years of a typical undergraduate chemical engineering curriculum (Rice & Do, 1995). In addition to these conservation principles, additional relationships called constitutive equations deduced from data are required to complete the model. To build such mechanistic or first principles models, the engineer must have some understanding of the physico-chemicalbiological mechanisms that govern the process. Typically, this is a difficult and long drawn process; however, when completed, such models can serve as a great proxy for the real process and can be exploited for optimal design and operation of the process. Alternatively, chemical engineers use experimental data to construct empirical data models ranging from simple linear regression models to the now wildly popular deep neural networks, which are relatively easy to develop (given sufficient quality data) but are usually limited in the range of their applicability as compared to the first principles based models. Increasingly popular is another class of models – hybrid models – which incorporate mechanistic approach (for phenomena that has been understood at a fundamental level) and empirical approach (for phenomena that is poorly understood as of now).

Also, in our choice of model structure, we need to ensure that the model does not contain terms that add little or no value to the understanding of the underlying behavior of the system or to the predictive capability of the model - i.e., the model should conform to the principle of parsimony. As a simple example, if we are seeking a model to relate a variable x (say temperature of a liquid stream) to a variable y (say composition of a particular chemical species in the liquid stream) and it is believed that the relationship is nonlinear. Would a quadratic model of the form y = a0 + a1 x + a2 x2 suffice? Or should a cubic term be included i.e., should a model of the form y = a0 + a1 x + a2 x2 + a3 x3 be employed? According to the principle of parsimony, the more complex cubic model should be chosen only when it offers a substantial advantage over the simpler quadratic model in predicting y using x values. Chemical engineering students must get enough practice in proposing appropriate model structures and in evaluating them so that they end up with the simplest and most suitable model that they can deploy for the intended purpose.

Fault detection

For the complex industrial process, it has become increasingly challenging to effectively diagnose complicated faults. A combined measure of the original Support Vector Machine (SVM) and Principal Component Analysis (PCA) is provided to carry out the fault classification, and compare its result with what is based on SVM-RFE (Recursive Feature Elimination) method. RFE is used for feature extraction, and PCA is utilized to project the original data onto a lower dimensional space. PCA, SPE statistics, and original SVM are proposed to detect the faults. Some common faults of the Tennessee Eastman Process (TEP) are analyzed in terms of the practical system and reflections of the dataset. PCA-SVM and SVM-RFE can effectively detect and diagnose these common faults. In RFE algorithm, all variables are decreasingly ordered according to their contributions. The classification accuracy rate is improved by choosing a reasonable number of features.

Process Identification and control

Process control is the study and application of automatic control in the field of chemical engineering. The primary objective of process control is to maintain a process at the desired operating conditions, safely and efficiently, while satisfying environmental and product quality requirements. Chemical process models which present the system behavior are useful in all phases of chemical engineering, from research and design to optimization and control and even plant operations

Generally, there are two major types of modeling approaches in chemical engineering, namely, mechanistic (white box, first principle) and AI-based approach like ANN and fuzzy logic methods. In the mechanistic approach, fundamental physical and chemical laws, such as conservation laws, construct the basis of the model. This approach contains algebraic and differential equations which involve mass, energy and momentum balances.

Due to the large number of variables affecting the process behavior and complex mathematical equations governing the system, many chemical processes are nonlinear and complicated. Consequently, it is hard and sometimes even impossible to present them by mechanistic models.

On the contrary, AI-based techniques have demonstrated their superb ability and have received much attention for chemical process modeling. The most common methods of AI for modeling purposes in chemical engineering are ANN and fuzzy logic, which sometimes are hybridized with evolutionary algorithms. In addition to ANN and fuzzy logic methods, their hybrid scheme named adaptive-network-based fuzzy inference system (ANFIS) which is actually a fuzzy inference system implemented in the framework of adaptive networks has also been applied for modeling purposes in chemical engineering.

Conclusion

The mathematics and engineering are interconnected in many ways, and that these interconnections cannot be understood properly from studies of how each of them is connected with technology. From the above data the artificial neural networks (ANN) has evolved for a diverse range of engineering applications such as data analysis, fault detection, signal processing, process modeling, and process identification and control.

In ANN, Mathematical modeling is a powerful tool for designing, predicting and understanding, processes and process equipment in the chemical industry, including the conservation of energy, material and momentum. ANNs are nonlinear empirical models that are particularly useful in presenting input-output data in order to predict the behavior of complex chemical engineering processes. They can also be used for data classification as well as image recognition. This are all the part of fuzzy logic and artificial neural network. So that fuzzy logic method and artificial neural network widely used in chemical engineering.

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