Artificial Intelligence in Membrane Science-A Review

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ABSTRACT. Artificial intelligence, which uses Artificial neural networks (ANN) are a powerful technique that has been used as a mathematical model to process information by receiving external inputs based on the structure's information and performing functional activities similar to those of biological neural network structures.The methods used in ANN involve non-parametric algorithms which are similar to and also mimic the cognitive functions of the human brain, for example, learning and problem-solving. Techniques based on ANN modelling are currently extensively used in a number of areas of chemical engineering, science, and technology, including water and wastewater treatment, for the simulation and optimization of complex problems. It consumes less time as compared to other models, viz. transfer models, which are quicker and much more reliable in computation for designing a membrane separation.

These are quite useful in cases where researchers do not have thorough feedback about the physical and chemical rules that govern systems as compared to other mathematical techniques which have been derived from applied linear algebra, such as principal component analysis (PCA). So, these tools are being used as powerful modelling tools that are applicable in the study of non-linear relationships between different features and parameters with great precision. ANN-based methods may be used in the determination of the complex relationship between input and output variables for optimising a process. In the present review, ANN modelling methods have been described that govern the estimation of membrane performance characteristics such as the permeate flux and rejection over the entire range of the process variables, such as feed concentration, temperature, pressure, pH, and superficial flow velocity, etc. These membranes are used in membrane separation such as nano filtration (NF), reverse osmosis (RO), microfiltration (MF), ultra filtration (UF), as well as in catalytic properties, extraction of metals such as nickel, etc. The data of ANN has been compared with other mathematical models such as response surface methodology (RSM) for the treatment of brackish water and green emulsion liquid membrane (GELM) used in the extraction of nickel from waste water.

Keywords. Chemical engineering; membrane; modeling; artificial neural networks; artificial intelligence; separation.

Introduction

Artificial intelligence (AI) or machine intelligence is a kind of intelligence shown by machines in contrast to natural intelligence which are displayed by animals including humans. It mainly includes the fabricating; designing and managing technology which is able in learning autonomously. It make decisions by own and performs the actions as per input of the data. AI consists of cluster of technology which includes software and hardware component. AI supports learning by machine, vision of computer by understanding and processing natural language.

With the help of (AI) in synthetic membranes incorporating as artificial neural networks(ANNs) methods haveused in study of the membrane phenomena. Artificial membranes have been used transport of inorganic/organic/biomolecules, so the scientist from different fields such as chemists, chemical engineers, biologists, pharmacologists, physicists and mathematicians have paid special attention the development of better membranes and theory which governs the transport phenomena during the last few decades. In Figure 1 the SEM images of the prepared reverse osmosis nano-composite membranes is shown. [[1- 7]. Since last few decades so many researches have also reported substantial works for separation of gas and liquid by using membrane technology

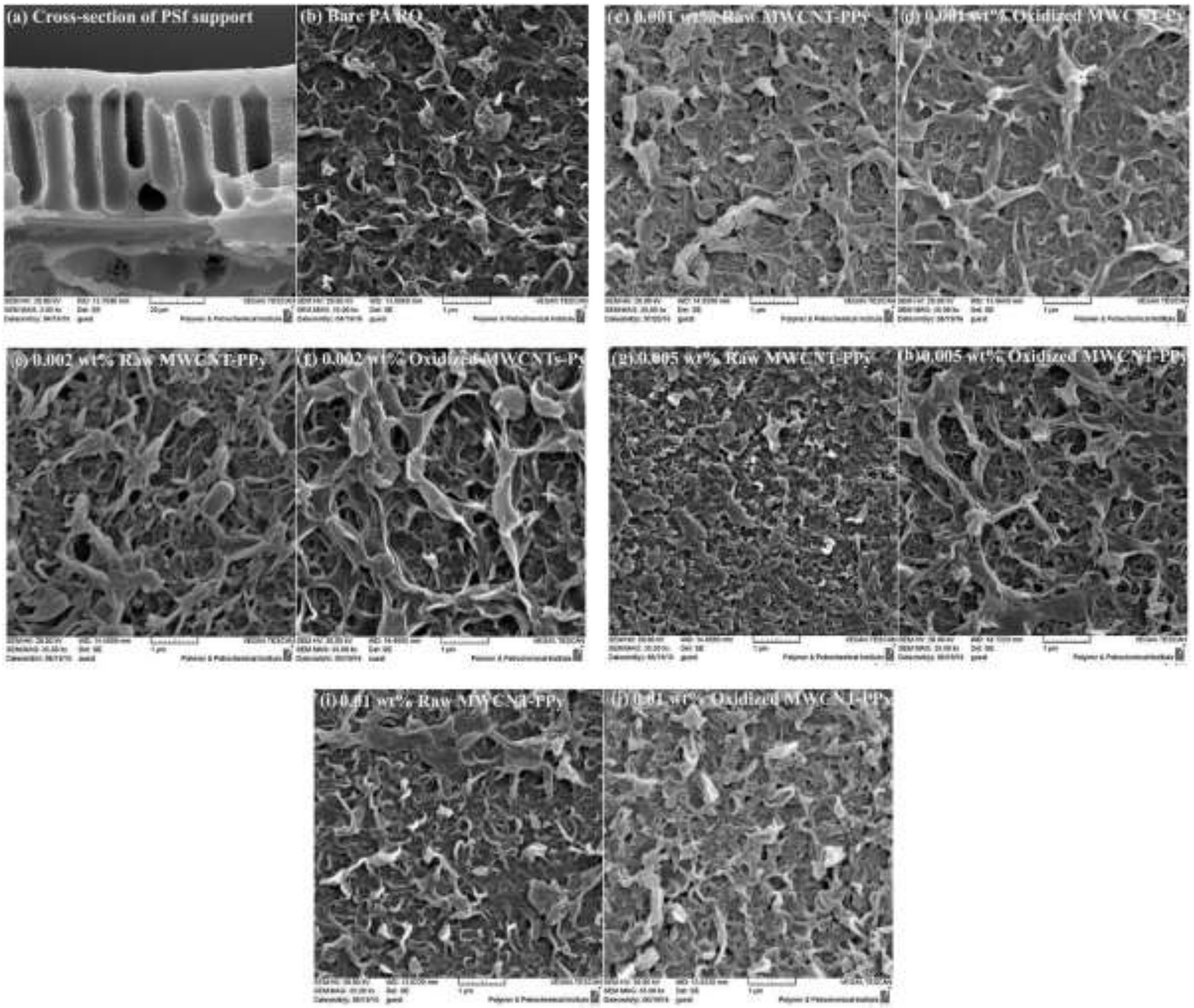

Figure 1. SEM images of the prepared reverse osmosis nano-composite membranes.

e.g.,seperations of some of the more prevalent gas from air, recovery of hydrogen and natural gas purification by using nonporous polymeric membranes. It provides high selectivity but poor permeability as compared to porous inorganic membranes which gives high permeability but poor selectivity. [8-10] But improvements in the membranes gavebetter results in terms of selectivity and permeability e.g., mixed matrix membranes (MMMs)which comprised molecular sieving materials embedded in polymer matrixes, have high potential performance for gas separation and the synthesis of the membranes are carried out by the combination of sol-gel reaction and polymerization to get desired the hybrid materials. [11-16]

In Artificial Neural Networks (ANN) which uses artificial intelligence, is a mathematical model where information are processed in response to external inputs given by the structure and functional parameters of synthetic membranes similar to biological neural network structures. In These models are made up of neurons and connections which are used mapping and coding/decoding of inputprovided by the membranes and output data. [Figure 2]

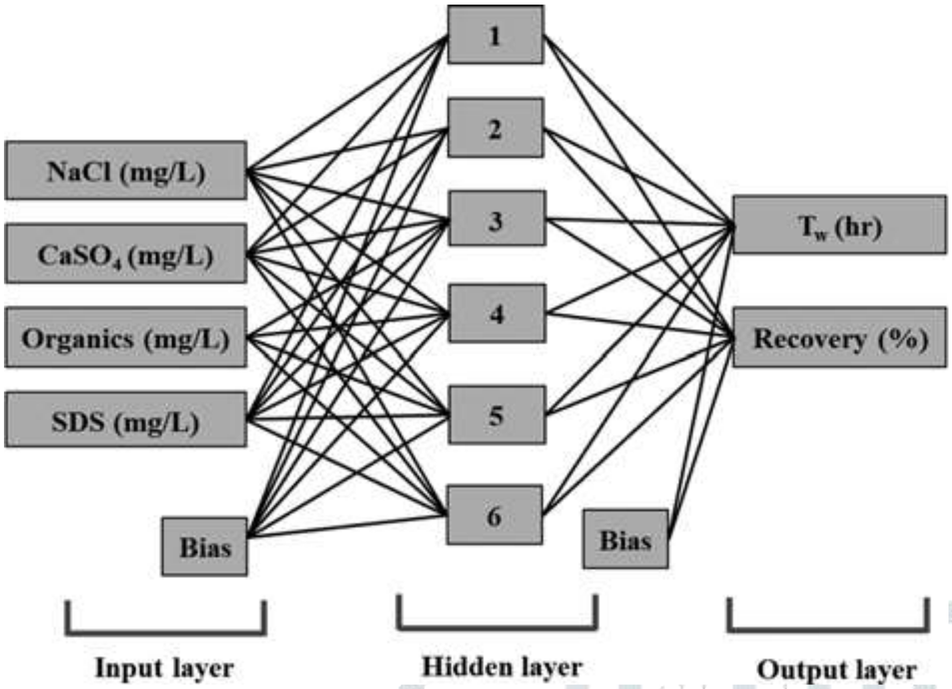

Figure 2. The schematic of the used ANN model.Adopted from B. Kim et al. Korean J. Chem. Eng., 2020, 37, (1), 1-10.[18].

ANNs methods have been used to predict the permeation flux and fouling resistance in ultrafiltration, nanofiltration and reverse osmosis membranes by using multi-layer perceptron (MLP) architecture which involves a feed forward type ANN as well as with Levenberg-Marquardt algorithm for the development of ANN. The accuracy of such model was found to be in acceptable limit as compared with experimental data and the value of minimum square error (MSE) was very low and correlation coefficient was near to 1. Neural network time series prediction methods have also been used in ANN to predict the performance of reverse osmosis membrane in a period of time that was unavailable with experimental data. [19] In ANN approach, it is not always necessary to carry out an entire series of experiment to collect and verify separation data.

ANN model methods have also been used in nanofibres which are materials with immense potential application in many fields of technology and the value predicted by the ANN models weretested as well asvalidated with the experimental values reported in literature.Nano fibers, nanowires, and nano-rods structurally composed of one dimension have been synthesized by the simplest technique e.g., electrospinning. Two dimensional (2-D) and three dimensional (3-D) dimensional nanofibres have also been synthesized by many research groups with various morphologies by using electrospinning and the specific surface area of these nanofibers are quite high which are suitable in many applications including drug loading, solar cell energy, tissue engineering, cancer therapy, etc. The diameter of fiber controls the following properties viz. mechanical strength, electronic conductivity and specific surface area. [20-24]. By using ANN methods the diameter of nanofibres of polyethylene oxide synthesized by electrospinning has been regulated. The ANN techniques and response surface methodology (RSM) have been compared to predict the rates of production of poly (acrylonitrile) nanofibers which are synthesized by electrospinning. (RSM) is based on factorial,which is a mathematical and statistical technique are used in designing experiments. The RSM involves several processes and each process consists of developing a linear or quadratic polynomial function which adjusts the response according to the operating conditions.[25,26]. Poly (methyl methacrylate) PMMA which is a biocompatible polymer possessing good mechanical strength has been extensively explored in the field of catalysis, energy storage, corrosion, etc. The diameters of PMMA nanofibers which have been prepared by electrospinning and the electrosppining parameter on fiber diameters have been predicted by calculating the index of relative importance of the input parameters using ANN method [27-29].

2. Preparation of synthetic membranes.

Membranes synthesized/prepared in laboratory using suitable chemical are called as artificial/synthetic membranes, which have been carried out in the laboratory using different chemical/substances mainly ion exchange resins, inorganic substances, and polymers etc. Worker have also used different type of polymer membranes *viz.* cellulose acetate, polyvinyl chloride, polyvinyl acetate, polystyrene membrane, parchment supported membrane, inorganic precipitate membrane, ion exchanger membrane and cellophane membranes for preparations of synthetic membranes in various laboratories worldwide and used as per their requirements as in reverse osmosis, ultra filtration and micro filtration, for the separation of ions, particles, microorganism, micro-filtration, electro dialysis technique etc. [30-33] In literature different methods have been reported for the preparation of porous polymeric membrane films, such as sintering, stretching, track etching, phase inversion and molecular imprinting; out of these many methods last two methods are efficient one. Molecularly imprinted polymers (MIPs) represent a new class of materials having artificially created receptor structures [34-36], have attracted considerable interest of scientists and engineers involved with the development of chromatographic adsorbents, membranes, sensors and enzyme and receptor mimics. [37-40].

3. Characterizations of Synthetic Membranes.

Synthetic membranes which are prepared in laboratory are characterized by using the principles of chemical kinetics and thermodynamics to evaluate the recognition properties of the membranes. Most of the theories which have developed during the past few decades are used in describing and modeling transport phenomena in membranes. Each theory has its own merits and demerits under suitable boundary conditions to explain the transport phenomena and recognition properties of the membranes.

3.1Absolute Reaction Rate Theory

In this theory a membrane is considered as systems consisting of a series of potential barriers existing one behind the other, across which material must pass in order to cross the membrane. For crossing across the membranes, the permeating species must possess minimum amount of energy and if there are n-barriers, then the rate of diffusion across eachbarriers in forward direction is expressd as given in equation(1)

$V_f = \quad K_i\, Ci\lambda_i$ (molecules /cm^2) (1)

$K_j$stands for specific velocity or rate constant for crossing barrier *i*,

$C_i$is the concentration of the substance at the *ith* position in the membrane

and$\lambda_j$is the distance between the adjacent potential barriers.

According to the theory of absolute rate process

$$Kj = K\ (k\ T/h)\ exp\ (-AGi/\ RT) \qquad (2)$$

This theory of absolute rate predict the processof the transmission coefficient (K)which is given as shown in equation (2)

$$Kj = K\ (k\ T/h)\ exp\ (-AGi/\ RT) \qquad (2)$$

k is the Boltzmann constant,

h is the Planck constant ,

where *AGi,* is the free energy of activation necessary for crossing the barrier *i*.

So, the equations for diffusions happening in backward over the barrier $_i$, isexpressedas follows, equation(3)

$$V_b = (K)^1 i+1.Ci+1.\ \lambda i +1 \qquad (3)$$

Hence, the total rate of diffusion which is also known as flux (J) will be expressed as

$$J= Ki\ Ci\lambda i-(K)^1 i+1.Ci+1.\ \lambda i +1 \qquad (4)$$

By assuming, $Ki= (K)^1 i+1=K$

and$\lambda i = \lambda i +1 =\lambda$

Then,

The value of $J = K\lambda(Ci\text{-}Ci+1) = K\lambda^2(Ci\text{-}Ci+1)/\lambda = K\lambda^2 dc/dx$ (5)

Here, the diffusion coefficient (D) = K λ^2

Several investigators have tested and verified the theory of absolute reaction rate in explaining the diffusion process which is occurring across synthetic membranes. These theories also explains the permeability of membranes to weak as well as strong electrolytes, non- electrolytes under the driving forces of a concentration gradient, activity gradient, and external and internal potential gradients and has also been used in osmosis and reverse osmosis. Diffusion across membraneshas been treated as "activated state" or the "transition state" theory by the Zwolinski, Eyring and Reese. [41]

3. Role of thermodynamics and kinetics in MIP

The optimized recognition properties of MIP is easily better explained by the Thermodynamic and kinetic considerations which is important in template/ligand binding in MIPs and the laws of the thermodynamics governs it. The change inenthalpy and entropy are highly correlated during molecular recognition event during the preparation of MIPs and recognition of templates by the MIPs. It also contributes to the observed differences of thermodynamic results during. The enthalpy and entropy changes during MIP binding/rebinding events have also contributed in molecular .Scientists have also calculated the change in Gibbs free energy and changein ΔG_{bind} of complex describing molecular recognition along with the kinetics parameters. [42-44].

4. Characterization of Membrane.

4.1 Membrane Morphology by Scanning electron Microscope (SEM)

Scanning electron (SEM) micrographs have been frequently used to characterizethe membrane after its preparation/development in various laboratories by the different investigators. It provides the details studies of the composite pore structure, micro/macro porosity, homogeneity, thickness, cracks and surface texture/morphology [45,46]. The information obtained from microscopic photographs/images has been useful in providing and also guiding in the preparation of well-ordered precipitates and/or crack free desired membranes.

4.2Characterization of Molecularly Imprinted Polymers

Despite different method available currently, the most common method which are being used in the characterization of MIPs are HPLC analysis, competitive ligand binding assays. MIPs have also been characterizes by the use of enantioselective chromatographic separation materials by utilizing enantioselective properties of MIPs/ and of receptors because enantiomers are most difficult to separate and require receptor sites capable of discriminating optical isomers.

So many other chromatographic studies encompassing quantitative and semi-quantitative have also been performed further investigate which influence the template basicity, hydrophobicity, as well as molecular shape along with selective recognition and binding properties in organic and aqueousprogens. [47-49].MIPs have also been characterized by using thermodynamics parameters where binding parameters' are usually estimated from Freundlich adsorption isotherms using mathematical models in saturation experiments and subsequently Scatchard analysis is carried out. [50-52]

4.3. Characterization of MIPs by Molecular modeling and computational approaches

Recently, the methods of combinational chemistry e.g. molecular modeling, molecular dynamics have been used in the optimization of synthesized MIPs. In molecular modeling, besides the choice of functional monomers, other factors e.g., type and amount of cross-linking agent, porogens, and polymerization conditions (e.g. temperature, pressure) may also be optimized and provides virtual libraries of functional monomers by screening the selected template against the designed library. [53]

The molecular dynamics methods involves the study of complex macroscopic systems or processes where involve replications of the small investigated systems. More recently, combinatorial libraries of MIPs have been prepared and it is used for the screening for high affinity and selectivity to the selected template analytesby using semi-automatic approaches. By using the automated procedures for MIP synthesis which enables at a small scale high-output preparation and screening of MIPs. So, testing of the compatibility between a variety of functional monomers and a given template in a library approach is easily achieved. [54,55].

6. Application of artificial intelligence.

6.1. In membrane distillation(MD) Themathematical and statistical technique is involved in the Response surface methodology (RSM) method for designing a particular experiments and it is based on factorial design involves. The different process of RSM method consists of developing a linear or quadratic polynomial function which adjusts the response as per the operating conditions. RSM along with ANN models have been applied for the prediction of wetting in a membrane distillation (MD) process used in the treatment of wastewater and RSM has been used to predict the wetting behavior of a MD process as functions of the operating variablesparametres which include the concentrations ofdifferent electrolytes e.g. NaCl, $CaSO_4$, organics materials such as humic acid 50%, Alginate 50%, and surfactants sodium dodecyl sulfate (SDS). [Table 1] summarizes the designed variables used for the experimental design.

Table 1. Experimental data used for RSM and ANN modelling.[18].

Run	Used in RSM	NaCl(mg/L)	CaSO4 (mg/L)	Organic (mg/L)	SDS(mg/L)	Time of wetting occurance (T_w)	Max.recovery of permeate (R_{max})
1	No	100,000	1,000	0	0	52.2	59.16
2	No	100,000	2,000	0	0	44.0	64.34
3	Yes	100,000	1,500	50	6	16.7	20.89
4	No	100,000	1,000	100	12	2.8	2.11
5	No	100,000	2,000	100	12	2.6	2.15
6	No	125,000	1,250	25	0	41.0	54.49
7	No	125,000	1,250	75	0	35.7	39.11
8	No	125,000	1,750	25	0	37.4	40.23
9	No	125,000	1,750	75	0	37.3	42.52
10	Yes	125,000	1,250	25	3	37.0	48.99
11	Yes	125,000	1,250	75	3	39.8	50.68
12	Yes	125,000	1,750	25	3	40.1	47.84
13	Yes	125,000	1,750	75	3	42.0	53.81
14	Yes	125,000	1,250	25	9	1.9	2.05
15	Yes	125,000	1,250	75	9	1.8	2.15
16	Yes	125,000	1,750	25	9	2.3	2.60
17	Yes	125,000	1,750	75	9	2.3	2.44
18	No	125,000	1,250	25	12	2.5	2.02
19	No	125,000	1,250	75	12	2.5	2.20
20	No	125,000	1,750	25	12	2.0	1.85
21	Yes	150,000	1,500	50	0	31.0	43.81
22	No	150,000	1,500	50	3	7.6	10.07
23	Yes	150,000	1,000	50	6	6.2	5.95
24	Yes	150,000	1,500	0	6	9.4	14.08
25	Yes	150,000	1,500	50	6	4.9	7.15

It is also reported that hydrophobic microporous membranesdo prevent the passage of feed solution but allow the transport of vapour distillate. [Figure 3]

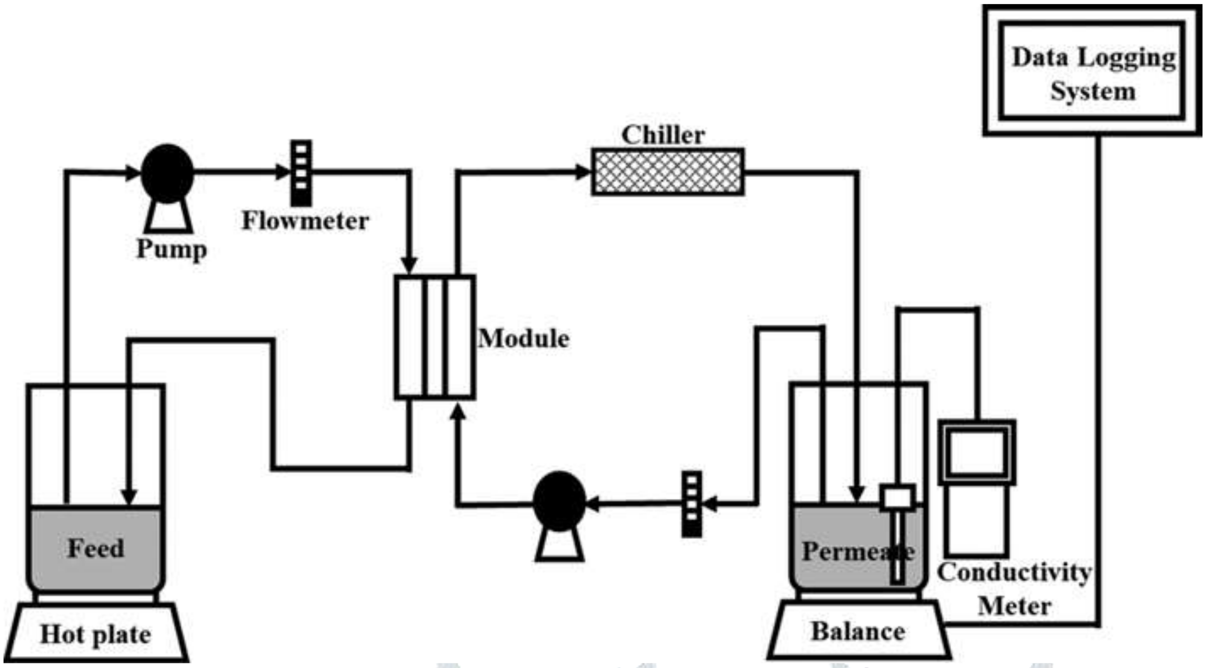

Figure 3.Schematic diagram of laboratory-scale DCMD system. Adopted from B. Kim et al. Korean J. Chem. Eng., 2020, 37, (1), 1-10.[18].

6.2 Application of ANN in study water flux in membrane using multi walled carbon nanotubes.

Prediction of the membrane problems such as of water flux which has been solved by the use of ANNsmethods and genetic algorithm [56]. So many studies have been conducted by using ANN and the results predictthat permeation flux and fouling resistance in ultrafiltration, nanofiltration and reverse osmosis membranes is with in precision.

Multi-layer perceptron (MLP) architecture, a feed forward type of NN has been utilized along with the Levenberg-Marquardt algorithm to fabricate the ANN methods and the accuracy of model was found to be in acceptable as compared with experimental data with minimum square error (MSE) .[Figure 4]

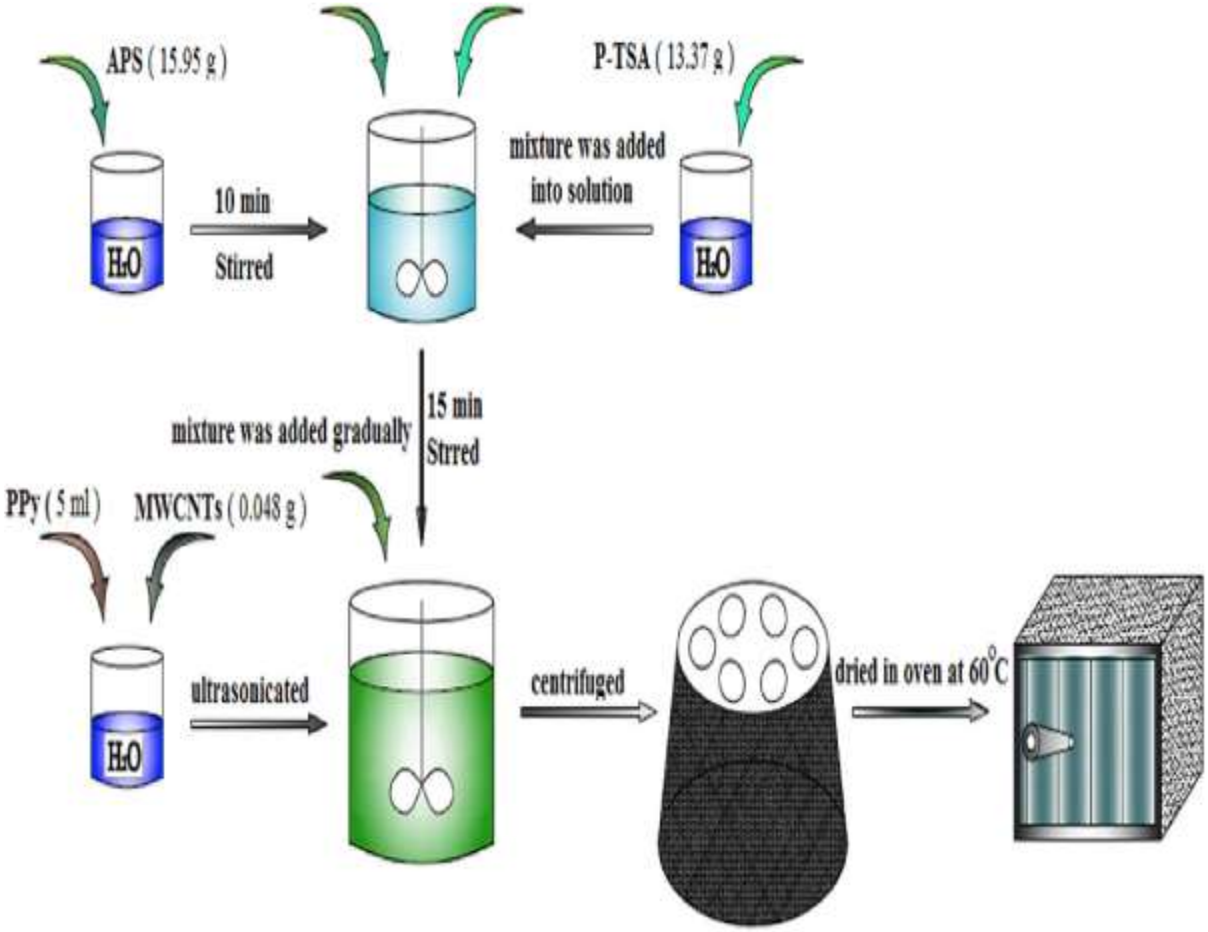

Figure 4. Process of preparing MWCNTs-PolyPyrrolenanocomposite (Adopted from J. Farahbakhsh, etal, Journal of membrane scince,2019,581,123-138).

Due to of nanoscale dimension of multi-walled carbon nanotubes (MWCNTs) possessing high porosity i.e. more surface area which exhibits the Improvements in water flux, salt rejection and fouling performance in (MWCNTs) materials hence they are used as an effective modifier in membrane technology.They are also commonly used in bio medicals materials.The solubility polyamide of (PA) layer in water have been significantly enhances due to the hydrogen bonding [Figure 5] in functionalized multi-walled carbon nanotubes and their hydrophilic surface assists in increasing water flux as well diffusion mechanism. [57-59].

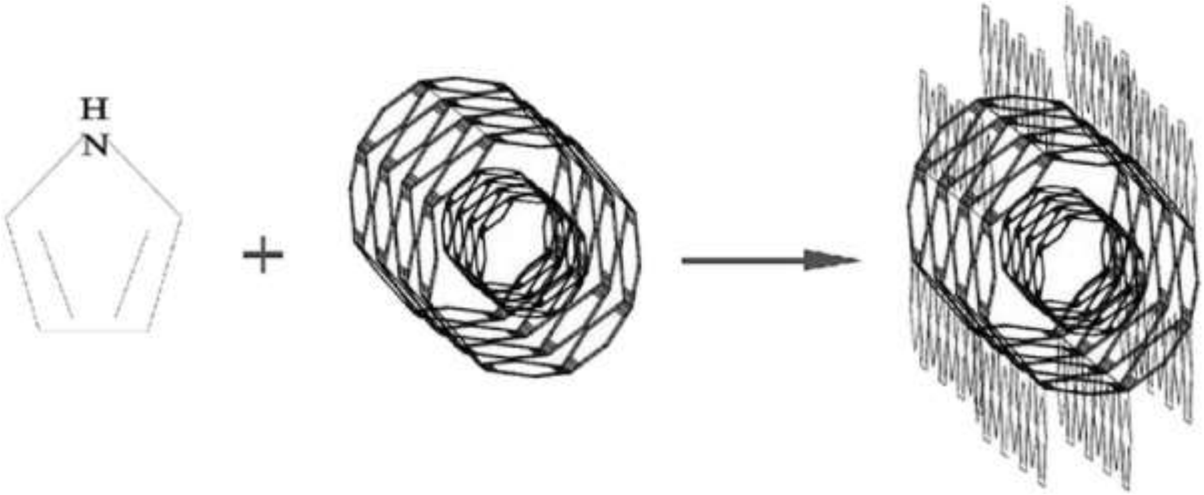

*Figure5.**C**onceptual schematic shape of MWCNTs-PolyPyrrole for hydrophilicity. (Adopted fromJ. Farahbakhsh, etal, Journal of Membrane Science,2019,581 123–138)[69].*

6.3 Application of Artificial neural network for membrane disc catalysts.

ANN methods have been used to predict an effective additive to the disc catalyst Co/SrCO3 catalyst which is used in the oxidation of CO in H_2along with other ten metals such as (X = B, K, Sc, Mn, Zn, Nb, Ag, Nd, Re and Tl) used as promoters for the catalytic activities of Co + X/SrCO3 catalyst and 16 physicochemical properties of those ten elements such as melting point, heat of vaporization, ionic radius, electronegativity, and so on have also been predicted by the ANN methods.An impregnation method has been used to prepare the disc catalysts in each catalyst. [Figure 6,7]

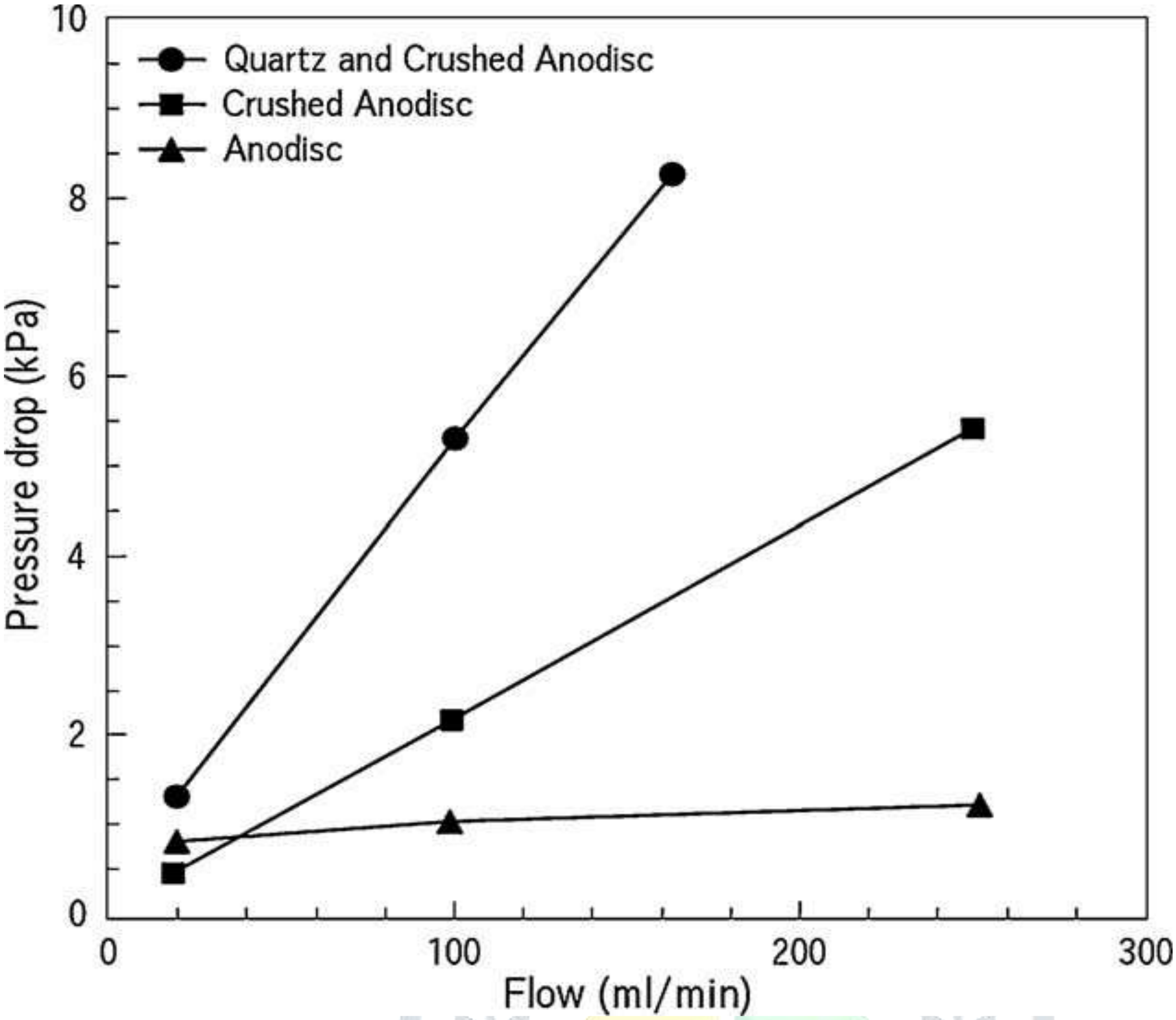

Figure.6 Effect of reaction temperature on catalytic activity of Ni/ Anodisc at 0.1 MPa, V/ F ¼ 25 ms. (Adopted from K. Omata et al. / Applied Catalysis A: General, 2009, 362, 14–19).

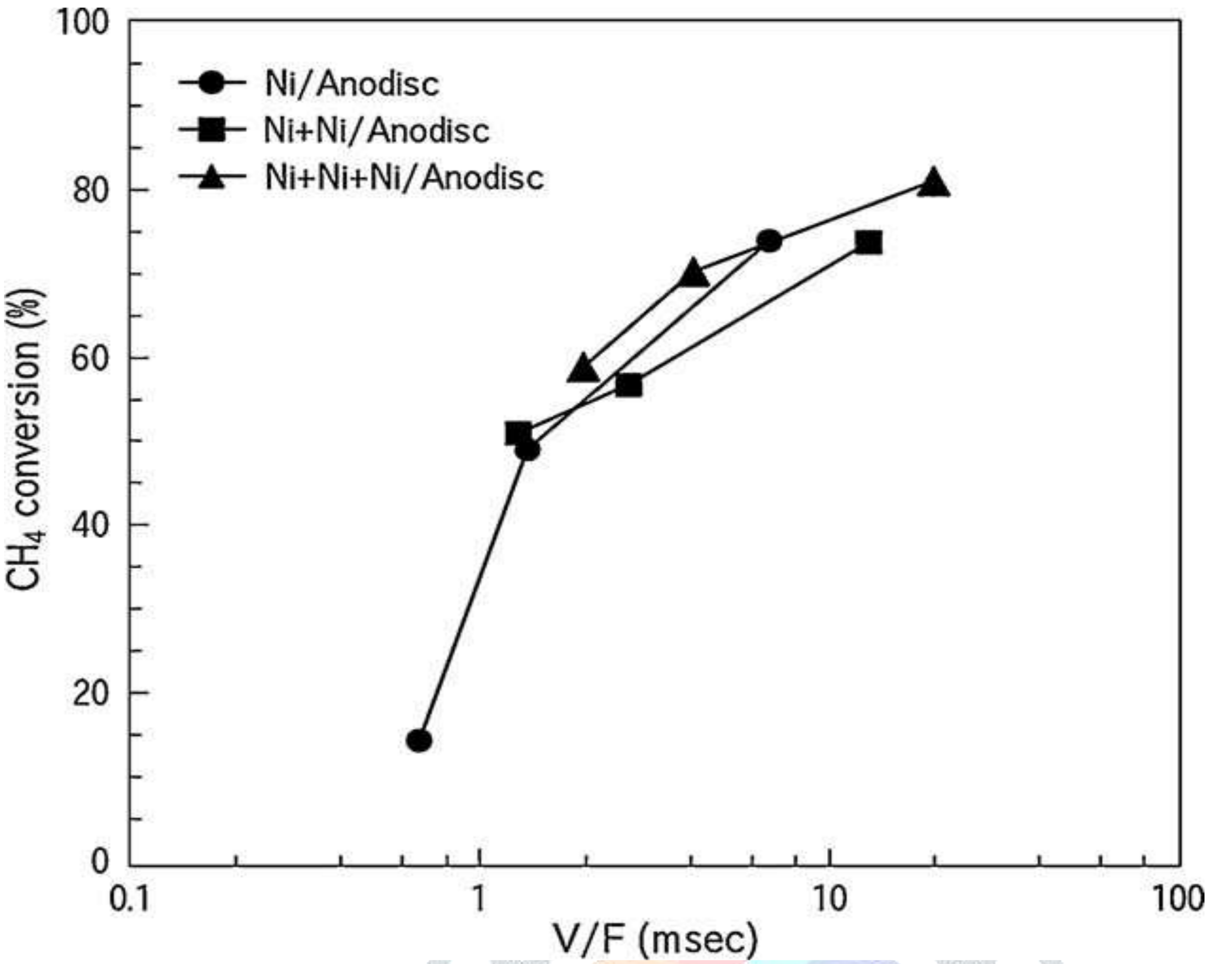

Figure 7.Effect of overlapping order of Ni/ Anodisc and Co-Mg / Anodisc at 973 K, 0.01 M Pa. (Adopted from K. Omata et al. / Applied Catalysis A: General,2009, 362, 14–19)[68].

MWCNTs have also been used water desalination and ANN techniques are utilized in studying the antfouling properties of the polymeric membranes by dispersing MWCNTsin it during the polymerization by using low viscosity monomers such as like pyrrole, cetyltrimethyl ammonium bromide, polydimethylsiloxane and hydroxyapatite-silicon and the result have found to be better with the functionalized MWCNTs. [60-63]The membrane problems for example prediction of water flux have been predicted by the ANN technique and genetic algorthim and recently NN have also been utilized in these cases. [64]

ANN model have been utilized in the extraction of the metal ions present in environment which serious concern and the data has been compared with response surface methodology (RSM). [65-66]Extraction of heavy metals ions such as Ni^{+2} present in wastewater and aqueous solution with emulsion liquid membrane (ELM) has been done by the use of Liquid membrane technology (LMT) which has emerged as suitable technique as compared to traditional liquid-liquid extraction since it provide high interfacial area and able to recover solute selectively.In the extraction of metal ions from polluted water with ELM by using LMT extraction and stripping of metal ions are achieved in single step with the use of surfactant, co-surfactant, and emulsifier etc. which stabilize emulsion droplets. [67].

Conclusion.

Artificial Intelligence or machine learning is a very popular emerging field of the science which is widely used in membrane technology.Software technologies are used in AI which design a robot/ a computer and perform works as like a human think and act.In biological systems as like human where more than 10^{11} nerves cell commonly known as neurons are interconnected and performs and control all the bodily and physiological activities by responding to the external and internal stimulus. Similar to these human behaviors of learning, the ANNs methods also uses the artificial intelligence (AI) as compare to intelligence in human which is natural) is used by the training dataset which set the values of inter-neuron connection as weights between processing elements similar to neuron. In the last the output network is able to approximate given response as a data.

Human brain learns things through experience and then simulates them for the next events. Inspired by human learning system, the ANN basically composed of three elements, learns the training dataset by setting the values of inter-neuron connection strength (weights) between processing elements (neuron) until the output network is able to approximate targets data. [28] Most of the membrane fouling studies has been done by utilizing the artificial intelligence (AI) as ANNs.[68] There have been some other efforts where ANNs has been used in combination with other methodology by mathematical and computational intelligence techniques which describe the process successfully and precisely which are able in processing nonlinear relationships between inputs data and outputs response [25] [29].

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