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Prediction of Liquid Detergent Properties using Artificial Neural Network

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Abstract : Neural networks have the potential to derived meaning from complicated or imprecise data. They can be used to extract patterns and detect trends, which are too complex to be notice by either humans or other computer techniques. A trained neural network can be thought of as an "expert" in the category of information it has been given to analyse. This expert can then be used to provide projections of given new situations of interest and answer "what if" question. Artificial network can be effectively used in various fields for different purposes. In this study, liquid detergents based on polymeric surfactant alkyd resin were formulated, analysed for various properties like foam volume, percent detergency and surface tension. The generated experimental data was used for training of feed forward artificial neural network with back propagation technique. The trained artificial neural network model was used for prediction of detergent properties. The result shows that artificial neural network is an excellent option modeling of such experimental data.
Keywords : Artificial neural network, ANN, liquid detergent, properties.

Mcculloh & Pitts[1] are pioneer of Artificial Neural Network (ANN) which has its fundamentals in reach interdisciplinary history from the early 1940s. Hebbs[2] put forward a learning scheme to relocate the synaptic strength between neurons. His 'postulate of learning' which is also known as 'Hebbian learning', which presented that the information can be stocked in synaptic connections and strength of synapse would raise by the repeated activation of neurons by the other ones across that synapse. Rosenblatt[3] & Block et al [4] gave rise to neuron like element called 'perceptron' & its learning procedure. There perceptron conversion procedure which is renewed form and more feasible over 'Hebb rule' for changing synaptic connection. Minsky & Peppert[5] have given the limitations of the single level perceptron. Nileson[6] recommended that the Multilayer Perceptrons (MLP) can be used to separate pattern nonlinearly in a hyperspace and in single layer perceptron, the perceptron convergence theorem should be used. Rumelhart et al[7] has demonstrated the conceptual basis of the back propogation which can be surely reminded as a revolutionary step put forward, which no one has previously

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done. Flood & Kartem[8] reviewed various applications of ANN in civil engineering, Dougherty[9] reviewed application of ANN in transportation engineering. Godbole[10] reviewed applications of ANN in wind engineering, Gardner & Dorling [11] reviewed applications of ANN in atmospheric sciences and concluded that the neural networks generally give as good or better results than linear methods. Z V P Murthy & M M Vora[12] applied the neural networks to simulate the separation of NaCl-H_2O system by reverse osmosis. S L Pandharipande et al[13,14,15&16] optimized ANN architecture for shell and tube heat exchanger, modeling of packed column, modeling of three phase inverse fluidized bed and formulation of detergents. In this work, the liquid detergent samples are prepared by using alkyd resin and other ingredients. The samples are tested for foam and percent detergency and surface tension. This experimental data is used for training of ANN. Herein, an attempt is made to highlight the use of ANN as a tool in modeling of detergent properties so that optimum detergent formulation can be decided.

Artificial Neural Network

ANNs are so called as they are made to behave like the network of neurons in human being. The most common for chemical engineering application is Multilayer ANN / Multilayer Perceptron (MLP) is made up of input layer, one or more hidden layers and an output layer, with nodes in each layer connected to other nodes in neighboring layers [17,18].Theout put of a node is scaled by connecting weights and fed forward to as input to the nodes in next layer of the network implying a direction of information processing. Hence MLP is also known as feed-forward neural network[19]. The hidden nodes pass the net activation through a nonlinear transformation function, such as the logistic sigmoidal or hyperbolic tangent to compute their outputs. For the training of such a MLP error back propagation algorithm suggested by Rumelhart is popular. The training of ANN is a similar to the learning of a child. The network learns, from patterns of data it is presented with. The trained network can be tested using new sets of data. The network is then corrected for any error in prediction. The final model developed by the ANN is independent of the underlying mechanism of the process.

The network process, new data using the mathematical correlation, developed during the course of training [20,21]. The ANNs must pass through three phases[22-24], training or learning phase, the recall phase, and the generalization phase.

The training phase is the learning period of the network. This is done by identifying the pattern in the data fed to the network. This information about the data pattern is stored by the network in the form of variables called weights and bias. The recall phase is the testing of new data by the network based on the pattern recognized by it in training phase. To make the network more accurate, the network is subjected to minor changes. This is done in the generalization phase. Generally, numerically intensive techniques are used to correct the errors.

The main advantage of using ANN is their reliability and suitability for processing noisy, incomplete input signals [24-26]. An advantage of ANNs over empirical models is their ability to periodically update the input-output performance through on-line self-training. Lastly, ANNs are truly Multiple input Multiple Output (MIMO) systems, as they can map many independent variables. Hence, ANNs perform well in pattern recognition type of problems[27-29]. The basic unit of ANN is artificial neuron. Fig 1 shows a fundamental representation of an artificial neuron or processing element (PE)[24].

In Figure 1, various inputs to the network are represented by the symbol, x(n). Each of these inputs are multiplied by a connection weight. These weights are represented by w(n). In the simplest case, these products are simply summed, fed through a transfer function to generate a result, and then output. This process lends itself to physical implementation on a large scale in a small package. This electronic implementation is still possible with other network structures which utilize different summing functions as well as different transfer functions.

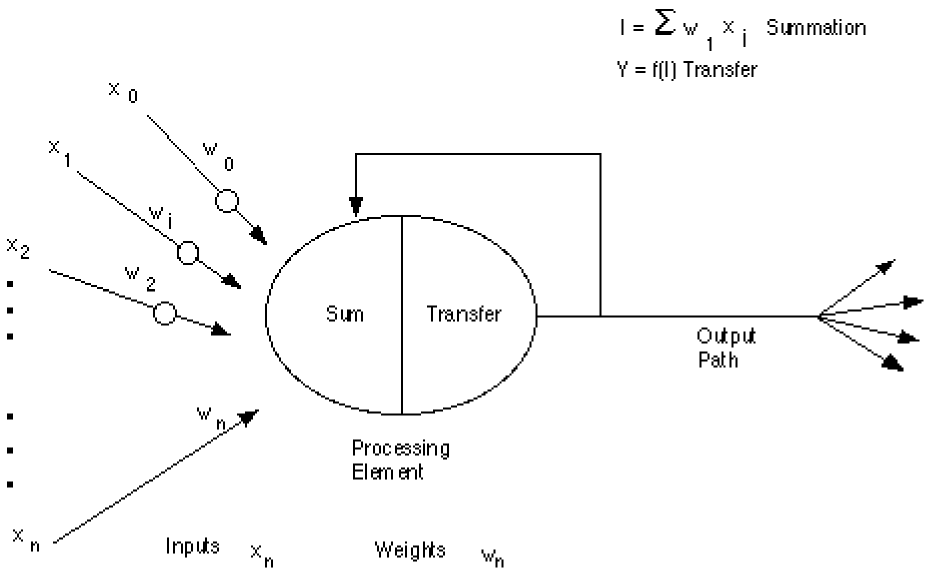

Fig. 1.A Basic Artificial Neuron.

Methods

Manufacture, analysis and testing of liquid detergent[30]

The formulation, analysis and testing of liquid detergents are performed by authors and details of procedure of experimentation are given elsewhere[31]. Liquid detergents (samples) are prepared using different concentrations of alkyd resin with sodium lauryl sulphate (SLS), PVA, sorbitol, EDTA and urea in a beaker (1l) with constant stirring (130-140 rpm/h) for 30 min (Table 1).The surface tension is measured using stalagnometer. Foam volume is measured by using mechanical agitation in a closed vessel method. Detergency test is performed using cotton cloth, soil medium, Washing of cloth was done in Terg-O-Tometer and reflectance is measured with an Elerepho reflection photometer with filter R-46 against an MgO-standard.

ANN training procedure

The ANN software used for present work is developed by Prof. S L Pandharipande & Yogesh Badhe[32] at Laxminarayan Institute of Technology; Nagpur.It is based on back propagation feed forward neural network, with three hidden layers. Some of the salient features of the software are as follows;

- Option for the selection of input & output nodes.
- Option for the selection of number of nodes in 1st,2nd& 3rd hidden layer.
- Data required for the learning can be inserted from file or keyboard.
- Option for the selection of suitable learning rate during running.
- Learning can be terminated at any value of error & frozen weights can be stored in a file, which can be used for further training.
- Use of three previous time elements for back propagation algorithms has made it more accurate.
- Has been successfully used for prediction, black box modeling, interpretation & recognition of industrial, research and experimental data.

The ANN requires a large database, both continuous and accurate, for training. In the present work, the ANN model is trained to Sum Square Error (SSE) of 0.0045 using Multilayer Perceptron trained with a nonlinear version of the Windrow-Hoff rule known as Generalized Delta Rule (GDR). Further training would still reduce the SSE to lower value. However, the possible danger of “over training” of the network may lead to incorrect prediction at lower SSE.

Table 1 – Composition of liquid detergents.								
Ingredients	**LD^1**	**LD^2**	**LD^3**	**LD^4**	**LD^5**	**LD^6**	**LD^7**	**LD^8**
SLS	7.00	6.00	5.00	4.00	3.00	2.00	1.00	0.00
Alkyd resin	0.00	1.00	2.00	3.00	4.00	5.00	6.00	7.00
SLES	5.56	5.56	5.69	5.56	5.56	5.56	5.56	5.56
Sorbitol	5.60	5.60	5.60	5.60	5.60	5.60	5.60	5.60
Urea	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
PVA	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
EDTA	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
NaOH	0.00	0.29	0.47	0.71	0.99	1.23	1.43	1.67
Water	77.73	77.49	77.27	77.03	76.75	76.51	76.31	76.07

Table 2 – Neural network topology for liquid detergent formulation						
Number of neurons				**Data Points**		
1st Hidden layer	**2nd Hidden layer**	**3rd Hidden layer**	**Output layer**	**Training**	**Test**	**Learning rate**
10	10	10	3	144	24	0.55
*First momentum factor: 0.75				*Second momentum factor: 0.01		
*Final error : 0.0045						

Table 3 – Data of LD^1& LD^3 used for training of ANN and predicted values

SLS	**Alkyd resin**	**SLES**	**NaOH**	**Water**	**Conc.**	**Time (min)**	**Foam volume (ml) Actual**	**Foam volume (ml) Predicted**	**% detergency Actual**	**% detergency Predicted**	**Surface tension (dy/cm) Actual**	**Surface tension (dy/cm) Predicted**
7	0	5.57	0	77.73	0.1	0	165	161.667	62.34	62.429783	45.601	45.5426
7	0	5.57	0	77.73	0.1	5	160	160.503	62.34	62.428274	45.601	45.5777
7	0	5.57	0	77.73	0.1	10	160	159.556	62.34	62.427006	45.601	45.6048
7	0	5.57	0	77.73	0.1	15	157	158.786	62.34	62.425935	45.601	45.6252
7	0	5.57	0	77.73	0.25	0	200	209.416	70.51	70.765737	35.81	35.8288
7	0	5.57	0	77.73	0.25	5	210	206.852	70.51	70.769992	35.81	35.8444
7	0	5.57	0	77.73	0.25	10	205	204.877	70.51	70.765752	35.81	35.8295
7	0	5.57	0	77.73	0.25	15	205	203.407	70.51	70.750925	35.81	35.7906
7	0	5.57	0	77.73	0.5	0	420	426.025	88.92	88.943413	31.32	31.3916
7	0	5.57	0	77.73	0.5	5	420	419.249	88.92	88.927904	31.32	31.354
7	0	5.57	0	77.73	0.5	10	420	413.325	88.92	88.918698	31.32	31.3116
7	0	5.57	0	77.73	0.5	15	400	408.263	88.92	88.91327	31.32	31.2683
7	0	5.57	0	77.73	1	0	635	628.145	92.47	92.463371	28.72	28.8698
7	0	5.57	0	77.73	1	5	630	628.04	92.47	92.467058	28.72	28.852
7	0	5.57	0	77.73	1	10	625	627.898	92.47	92.472491	28.72	28.8341
7	0	5.57	0	77.73	1	15	625	627.713	92.47	92.479633	28.72	28.8168
5	2	5.69	0.47	77.27	0.1	0	148	143.521	67.85	67.792127	45.02	44.9648
5	2	5.69	0.47	77.27	0.1	5	145	143.148	67.85	67.770886	45.02	44.995
5	2	5.69	0.47	77.27	0.1	10	142	142.831	67.85	67.753092	45.02	45.0246
5	2	5.69	0.47	77.27	0.1	15	138	142.559	67.85	67.738285	45.02	45.0537
5	2	5.69	0.47	77.27	0.25	0	185	184.448	75.89	75.537576	35.94	35.9811
5	2	5.69	0.47	77.27	0.25	5	182	182.333	75.89	75.524077	35.94	35.9681

5	2	5.69	0.47	77.27	0.25	10	181	180.579	75.89	75.51967	35.94	35.9565
5	2	5.69	0.47	77.27	0.25	15	180	179.114	75.89	75.523008	35.94	35.9466
5	2	5.69	0.47	77.27	0.5	0	300	298.605	88.39	88.338402	30.42	30.4778
5	2	5.69	0.47	77.27	0.5	5	300	296.451	88.39	88.336345	30.42	30.4774
5	2	5.69	0.47	77.27	0.5	10	295	294.747	88.39	88.331655	30.42	30.4719
5	2	5.69	0.47	77.27	0.5	15	291	293.382	88.39	88.323458	30.42	30.4634
5	2	5.69	0.47	77.27	1	0	480	479.782	91.92	91.914137	28.61	28.7655
5	2	5.69	0.47	77.27	1	5	475	477.31	91.92	91.933528	28.61	28.7562
5	2	5.69	0.47	77.27	1	10	475	475.063	91.92	91.947712	28.61	28.7488
5	2	5.69	0.47	77.27	1	15	470	473.098	91.92	91.957127	28.61	28.7432

Results and Discussion

The experimentation thus resulted in generation of 192 data samples. There are 7 input parameters, concentration of various ingredients namely alkyd resin 0-7.00%, SLS 0-7.00%, SLES 5.56-5.69%, NaOH 0.00-1.67%, water 76.06-77.73%. Here we have not considered the concentrations of sorbitol, urea and PVA, as they are constant. The 6th input parameter is concentration of detergent in water which is varied from 0.1-1.0%. The 7th parameter is time element from 0-15 min. Composition of liquid detergents is shown in Table 1.There are three output parameters namely foam volume, surface tension and percent detergency. The data is divided into two parts one having 144 data points as a training data points and 24 data points as testing data set. The training data of LD1 & LD3 is shown in table 3 while test data set is shown in Table 4. Predicted values for foam volume, %detergency & surface tension are also given along with the actual values in the table 3 & 4. Architecture of ANN used for prediction is given in Table 2. During the training phase, first a single hidden layer with 10 neurons is used. At this stage, it could not reach the requisite error goal. In the next step, second hidden layer with 10 neurons is used. But, this also could not meet the requirements. Finally, after all such combination, the present configuration is reached as it attained the required error goal. This final ANN architecture has three hidden layers with 10 neurons each. In the network of detergent formulation, the function used for PEs of input, hidden and output layers are "sigmoidal function ". Fig 2-12 represent comparison between predicted and actual values of foam volume, surface tension and percent detergency of various samples.

The comparison between predicted and experimental (actual) values of foam volume, surface tension and percent detergency indicates that the trained ANN can be successfully used as model for prediction of properties liquid detergents.

Every detergent industry spent large amount of money, time and manpower in their research and development work, where they have done many experiments on trial and error basis to obtain best detergent formulation. However, by using ANN one can predict the formulations and properties of detergents with the best performance. It will save money, time and manpower required for detergent industry and will make the product more economic.

Conclusion

Various liquid detergent formulations have been prepared and analyzed for foam volume, surface tension and percent detergency. The data generated was used for training of ANN. The important decision to be made is regarding composition of raw materials along with process parameters in such a manner such that the detergents are of high quality, i.e. good foam and high detergency. Presently, there is no such mathematical model developed which could address this problem. ANN, which is a black box modeling tool, has been tried and tested for modeling of formulation of detergent. The use of ANN for prediction of percent detergency, surface tension and foam volume is quite encouraging. There is close agreement between predicted experimental actual values. The software developed can be used to predict the properties without undertaking exhaustive experimental work. Thus this work can open up new horizons for computing the performance and composition of detergents.

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