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Modeling of Liquid-Liquid Extraction in Spray Column Using Artificial Neural Network

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Abstract- Liquid-liquid extraction is a process for separating the components of a liquid feed mixture by contacting with a liquid solvent phase. The operation is carried out in spray columns, packed beds, rotating disc contactors & plate columns. The effective rate of mass transfer is dependent upon several factors such as mass transfer coefficient, transfer area and magnitude of driving force applied. Multi Layer Perceptron (MLP) is a type of feed forward neural network applied to chemical engineering operations. Present work is aimed at developing ANN models with different topologies for liquid-liquid extraction carried in spray column for a system of acetic acid-water-benzene. The accuracy of the ANN model is dependent upon the number of hidden layers & number of neurons in each hidden layer. Artificial neural network models 1 & 2 are developed for modeling liquid-liquid extraction spray column, correlating mass transfer coefficient & mass transfer rate with flow-rate of extract phase , equilibrium concentration of acetic acid in aqueous phase & height of organic phase in column. The topology of the architecture was different for both the models. Based on results & discussions it can be concluded that both the models are successful in estimating the parameters but because of higher accuracy of estimation for both the training & test data sets ANN model 2 is more suitable. The work is demonstrative and the accuracy of estimation can be improved by altering the topology.

Index Terms- liquid-liquid extraction, spray column, modeling, artificial neural network, mass transfer coefficient

I. INTRODUCTION

Liquid-liquid extraction is a process for separating the components of a liquid feed mixture by contacting with a liquid solvent phase. The process takes advantage of differences in the chemical properties of the feed components, such as differences in polarity and hydrophobic or hydrophilic character, to separate them. The transfer of components from one phase to the other is driven by a deviation from thermodynamic equilibrium and the equilibrium state depends on the nature of the interactions between the feed components and the solvent phase. The potential for separating the feed components is determined by the differences in this interaction. The operation is carried out in spray columns, packed beds, rotating disc contactors & plate columns. The effective rate of mass transfer is dependent upon several factors such as mass transfer coefficient, transfer area and magnitude of driving force applied. The mass transfer coefficient for a spray column is a function of a number of parameters that include velocity of raffinate & extract phases, sparger specifications, drop size, contact height of column & column dimensions.

II. LITERATURE SURVEY

Artificial Neural Network

An Artificial Neural Network (ANN) is an information processing paradigm that is inspired by the way the biological nervous system, such as brain processes information. It is composed of large number of highly interconnected processing elements (neurons) working in unison to solve specific problem [1].

Multi Layer Perceptron (MLP) is a type of feed forward neural network applied to chemical engineering operations. It consists of multilayer hierarchical structure with input & output layers & has at least one hidden layer of processing units in between them. The layers between the input and output layers are termed "hidden" since they do not converse with the outside world directly. The nodes between the two successive layers are fully connected by means of constants called as weights. The outputs from nodes of input layer are fed to hidden layer nodes, which in turn, feed their outputs to the next hidden nodes. The hidden nodes pass the net activation through a nonlinear transformation of a linear function, such as the logistic sigmoidal or hyperbolic tangent to compute the outputs. For the training of MLP, error back propagation algorithm suggested by Rumelhart[2] is popular. This is based on a nonlinear version of the Windro-Hoff rule known as Generalized Delta Rule (GDR). The schematic of the typical MLP network used in developing ANN model in the present work is shown in fig 1.

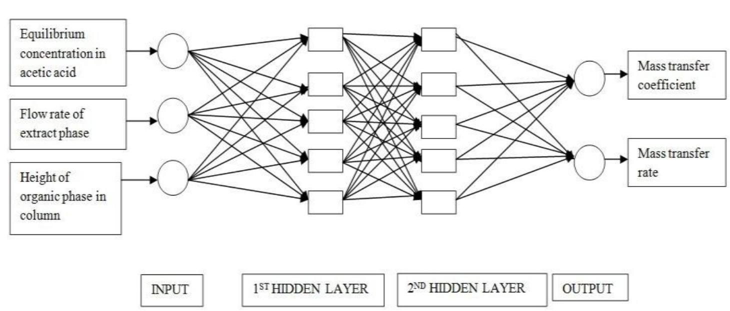

Figure no 1: Simple feed forward neural network with two hidden layer

Various applications of ANN are, an approach to fault diagnosis in chemical processes(3), fault diagnosis in complex chemical plants(4), incipient fault diagnosis of chemical process(5), leak detection in liquefied gas pipeline(6),(7), for estimation of mass transfer coefficient for fast fluidized bed solids(8), modeling of distillation column(9), detergent formulation(10), modeling of unsteady heat conduction in semi infinite solid(11), prediction of mass transfer coefficient in downflow jet loop reactor(12) and modeling of packed column(13) and similar other(14,15,16) were also reported.

Modeling of liquid-liquid extraction is a topic of interest among researchers & several papers have been reported in literature related to various aspects like modeling , simulation & control of liquid-liquid extraction columns(19), modeling mass transfer coefficient for liquid-liquid extraction with the interface adsorption of hydroxyl ions(17), a bivariate population balance simulation tool for liquid-liquid extraction columns(20), use of neural network for modeling of liquid-liquid extraction process in the rotating disc columns(21), multivariable control of a pulsed liquid-liquid extraction column by neural network(18). The present work is aimed at modeling liquid-liquid extraction spray column using artificial neural network. The experimental data generated for acetic acid-water-benzene system has been used. Mass transfer coefficient is estimated for variation in volumetric flow rate of extract phase, height of organic phase in the column and equilibrium concentration of acetic acid. It is also aimed to develop Artificial Neural Network model for correlating these sets of parameters for liquid-liquid spray extraction column.

III. MATERIALS AND METHODS

A. Generation of equilibrium data experimentally for the liquid-liquid extraction in spray column for a system of acetic acid-water-benzene.

B. Experimental set up for spray column

The schematic for the experimental set-up liquid-liquid extraction is as shown in figure no 2 .It consists of a glass tube of diameter & height 70 & 88 cm respectively. The sparger having diameter of50 mm is placed inside the column. Centrifugal pump is provided to supply the extract phase to the column. Three ball valves are provided for monitoring flow rates. Rota meter is provided for measuring the inlet flow rate of extract phase to spray column. A tank is mounted at the top of the assembly for steady supply of mixture of acetic acid and benzene to the spray column. A tank is provided for storage of extract phase at the bottom section of column.

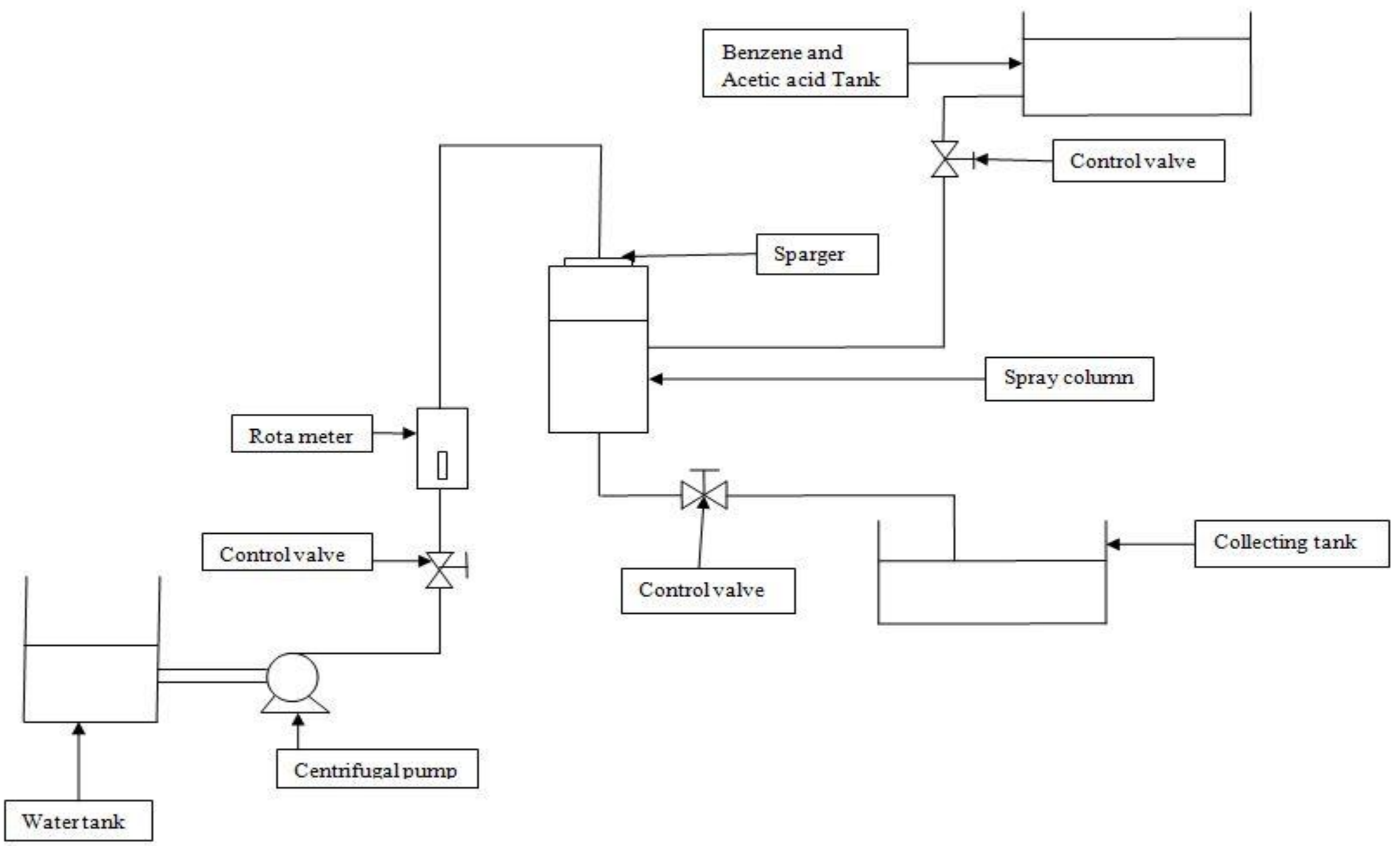

Figure no. 2: schematic for the experimental set-up of liquid-liquid extraction of spray column

Observations: The experimental data generated for various runs along with the calculated values of mass transfer coefficient and rate are given in table 1.

Table no 1: Experimental data

Sr no.	Equilibrium concentration of acetic acid (gmol/lit)	Height of feed in column (cm)	Flow rate (m^3/ sec) $1{\times}10^{-5}$	Mass transfer coefficient $1{\times}10^{-4}$ (sec^{-1})	Mass transfer rate $1{\times}10^{-4}$ (gmole/sec)
1	0.4901	50	3.33	1.78	1.66
2	0.4901	50	5	3.2	3
3	0.4901	50	6.66	5.13	4.8
4	0.4901	50	7.5	6.43	6
5	0.4901	55	3.33	1.68	1.73
6	0.4901	55	5	3.11	3.2
7	0.4901	55	6.66	4.8	4.93
8	0.4901	55	7.5	6.14	6.3
9	0.4901	60	3.33	1.6	1.8
10	0.4901	60	5	299	3.3
11	0.4901	60	6.66	4.51	5.06
12	0.4901	60	7.5	5.76	6.45
13	0.4901	65	3.33	1.58	1.93
14	0.4901	65	5	2.79	3.4
15	0.4901	65	6.66	4.28	5.2
16	0.4901	65	7.5	5.57	6.75
17	0.5769	50	3.33	1.56	1.73
18	0.5769	50	5	2.54	2.8
19	0.5769	50	6.66	3.74	4.13
20	0.5769	50	7.5	4.49	4.95
21	0.5769	55	3.33	1.48	1.8
22	0.5769	55	5	2.39	2.9
23	0.5769	55	6.66	3.63	4.4
24	0.5769	55	7.5	4.46	5.4
25	0.5769	60	3.33	1.46	1.93
26	0.5769	60	5	2.26	3
27	0.5769	60	6.66	3.52	4.66
28	0.5769	60	7.5	4.31	5.7
29	0.5769	65	3.33	1.39	2
30	0.5769	65	5	2.22	3.2
31	0.5769	65	6.66	3.44	4.93
32	0.5769	65	7.5	4.29	6.15
33	0.6035	50	3.33	1.61	1.86
34	0.6035	50	5	2.6	3
35	0.6035	50	6.66	3.93	4.53
36	0.6035	50	7.5	5.21	6
37	0.6035	55	3.33	1.52	1.93
38	0.6035	55	5	2.44	3.1
39	0.6035	55	6.66	3.78	4.8
40	0.6035	55	7.5	4.97	6.3
41	0.6035	60	3.33	1.48	2.06
42	0.6035	60	5	2.38	3.3
43	0.6035	60	6.66	3.66	5.06
44	0.6035	60	7.5	4.78	6.6
45	0.6035	65	3.33	1.46	2.2
46	0.6035	65	5	2.33	3.5
47	0.6035	65	6.66	3.56	5.33
48	0.6035	65	7.5	4.61	6.9

IV. DEVELOPING ARTIFICIAL NEURAL NETWORK MODELS 1 AND 2

This part of present work is devoted for developing artificial neural network model for the liquid-liquid extraction data generated experimentally.

The accuracy of the ANN model is dependent upon the number of hidden layers & number of neurons in each hidden layer. Artificial neural network models 1 & 2 having different topology are developed in the present work using elite-ANN(C).The details of architecture of topology of ANN models 1 & 2 is given in table 2. The total data set of 48 points is divided into two parts; training & test data set having 36 & 12 data points respectively as shown in table-2.

Table no. 2 Details of architecture of topology for ANN models 1 & 2

ANN model	No. of neurons					Data points	
	Input layer	1st Hidden layer	2nd Hidden layer	3rd Hidden layer	Output layer	Training data	Test data
ANN model-1	3	0	5	5	2	36	12
						RMSE error 0.01443	RMSE error 0.02933
ANN model-2	3	0	10	10	2	36	12
						RMSE Error 0.00704	RMSE Error 0.07008

The details of the output values of parameters mass transfer rate & coefficient for training & test data sets obtained by using ANN model -1 & model -2 are given in table -3 & 4.the iteration and the corresponding error during the training mode for developing ANN model 1 & 2 are plotted as shown in figure numbers 3 & 4.

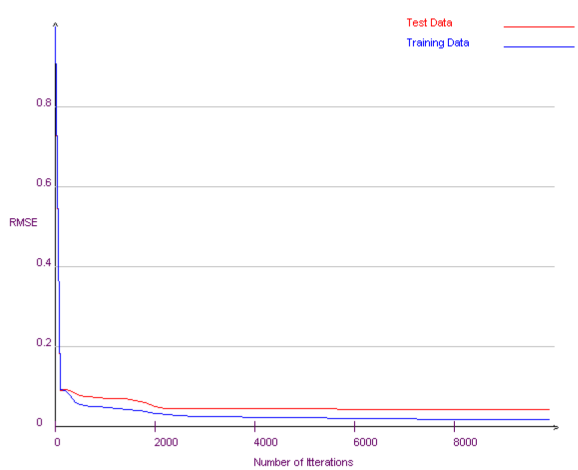

Figure no. 3: Iterations and the corresponding RMSE error for ANN model 1

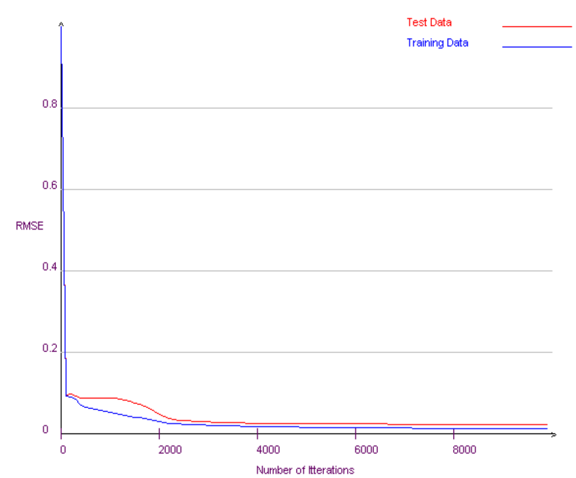

Figure no.4: Iterations and the corresponding RMSE error for ANN model2

Table no 3: Output values of parameters mass transfer rate & coefficient for training data sets predicted by using ANN model - 1 & model - 2

Sr no	Equilibrium concentration	Height of column	Flow rate	Mass transfer coefficient	Mass transfer rate	Predicted output mass transfer coefficient for ANN model 1	Predicted output mass transfer coefficient for ANN model 2	Predicted output mass transfer rate for ANN model 1	Predicted output mass transfer rate for ANN model 2
1	0.4901	50	5	3.2	3	3.225	3.177	3.019	3.057
2	0.4901	50	6.66	5.13	4.8	5.219	5.176	4.775	4.779
3	0.4901	50	7.5	6.43	6	6.285	6.291	6.074	6.029
4	0.4901	55	3.33	1.68	1.73	1.583	1.612	1.823	1.837
5	0.4901	55	6.66	4.8	4.93	4.734	4.795	4.993	4.937
6	0.4901	55	7.5	6.14	6.3	6.076	6.122	6.218	6.254
7	0.4901	60	3.33	1.6	1.8	1.565	1.574	1.833	1.833
8	0.4901	60	5	2.99	3.3	2.965	2.926	3.221	3.237
9	0.4901	60	7.5	5.76	6.45	5.775	5.792	6.432	6.491
10	0.4901	65	3.33	1.58	1.93	1.547	1.553	1.850	1.839
11	0.4901	65	5	2.79	3.4	2.821	2.833	3.428	3.430
12	0.4901	65	7.5	5.57	6.75	5.641	5.547	6.671	6.717
13	0.5769	50	3.33	1.56	1.73	1.548	1.565	1.870	1.824
14	0.5769	50	6.66	3.74	4.13	3.810	3.739	4.020	4.095
15	0.5769	50	7.5	4.49	4.95	4.672	4.573	4.875	4.933
16	0.5769	55	3.33	1.48	1.8	1.547	1.544	1.895	1.842
17	0.5769	55	5	2.39	2.9	2.414	2.420	2.866	2.824
18	0.5769	55	7.5	4.46	5.4	4.497	4.411	5.391	5.359
19	0.5769	60	3.33	1.46	1.93	1.542	1.539	1.924	1.880
20	0.5769	60	5	2.26	3	2.358	2.312	3.019	2.987
21	0.5769	60	7.5	4.31	5.7	4.332	4.284	5.819	5.771
22	0.5769	65	5	2.22	3.2	2.276	2.221	3.192	3.185
23	0.5769	65	6.66	3.44	4.93	3.401	3.510	4.935	4.869
24	0.5769	65	7.5	4.29	6.15	4.277	4.231	6.235	6.184
25	0.6035	50	3.33	1.61	1.86	1.557	1.570	1.931	1.864
26	0.6035	50	5	2.6	3	2.529	2.611	3.046	2.986
27	0.6035	50	7.5	5.21	6	5.049	5.157	6.107	6.001
28	0.6035	55	3.33	1.52	1.93	1.553	1.554	1.956	1.912
29	0.6035	55	5	2.44	3.1	2.465	2.442	3.139	3.132
30	0.6035	55	7.5	4.97	6.3	4.947	4.977	6.336	6.323
31	0.6035	60	5	2.38	3.3	2.393	2.276	3.238	3.314
32	0.6035	60	6.66	3.66	5.06	3.689	3.707	5.104	5.087
33	0.6035	60	7.5	4.78	6.6	4.808	4.800	6.478	6.540
34	0.6035	65	3.33	1.46	2.2	1.538	1.569	2.008	2.151
35	0.6035	65	6.66	3.56	5.33	3.604	3.496	5.382	5.347
36	0.6035	65	7.5	4.61	6.9	4.737	4.682	6.621	6.699

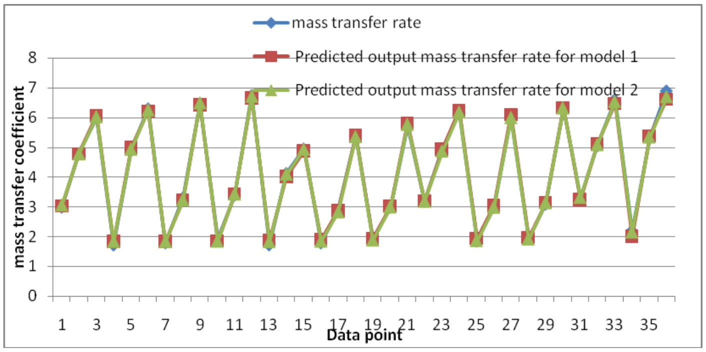

Figure no 5: Comparison of actual and predicted mass transfer coefficient obtained by ANN model 1 & model 2 for training data

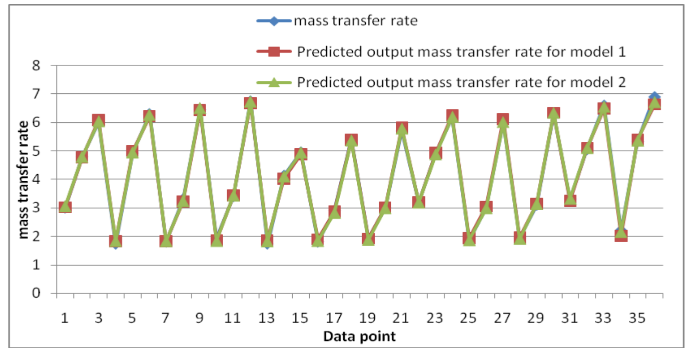

Figure no 6: Comparison of actual and predicted mass transfer rate by ANN model 1 & model 2 for training data

Table no. 4: Output values of parameters mass transfer rate & coefficient for test data sets predicted by using ANN model 1 & model 2

Sr no	Equilibrium concentration	Height of column	Flow rate	Mass transfer coefficient	Mass transfer rate	Predicted output mass transfer coefficient for ANN model 1	Predicted output mass transfer coefficient for ANN model 2	Predicted output mass transfer rate for ANN model 1	Predicted output mass transfer rate for ANN model 2
1	0.4901	50	3.33	1.78	1.66	1.601	1.676	1.818	1.850
2	0.4901	55	5	3.11	3.2	3.094	3.043	3.091	3.111
3	0.4901	60	6.66	4.51	5.06	4.510	4.447	5.296	5.166
4	0.4901	65	6.66	4.28	5.2	4.482	4.221	5.752	5.481
5	0.5769	50	5	2.54	2.8	2.458	2.535	2.725	2.720
6	0.5769	55	6.66	3.63	4.4	3.606	3.703	4.238	4.343
7	0.5769	60	6.66	3.52	4.66	3.465	3.617	4.508	4.603
8	0.5769	65	3.33	1.39	2	1.534	1.544	1.958	1.951
9	0.6035	50	6.66	3.93	4.53	4.145	4.011	5.077	4.593
10	0.6035	55	6.66	3.78	4.8	3.884	3.898	5.046	4.838
11	0.6035	60	3.33	1.48	2.06	1.547	1.556	1.981	2.002
12	0.6035	65	5	2.33	3.5	2.298	2.139	3.355	3.498

V. RESULTS AND DISCUSSION

Graphs are plotted between the actual and predicted values of output parameters mass transfer coefficient and mass transfer rate obtained by using ANN model 1 & 2, for training data set as shown in figure no. 5 & 6 respectively. It can be said that the actual & predicted values are close to each other. Both the ANN models 1 & 2 have high accuracy levels of prediction.

Similarly graphs are plotted between the actual and predicted values of output parameters, mass transfer coefficient and mass transfer rate respectively for test data set for ANN model 1 & 2 as shown in figures 7 & 8 respectively. It can be said that the actual & predicted values are close to each other.

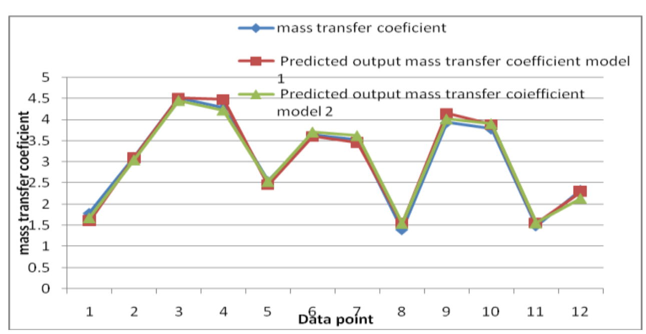

Figure no 7: Comparison of actual and predicted mass transfer coefficient obtained by ANN mode -1 & model -2 for test data set

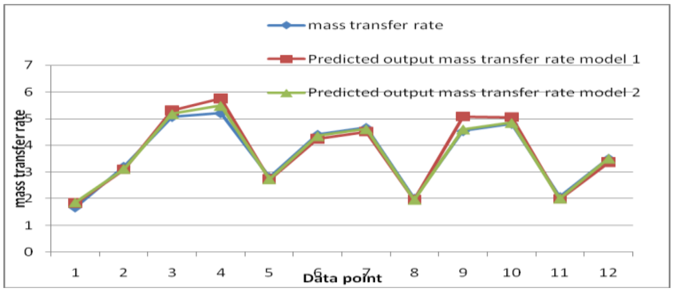

Figure no 8: comparison of actual and predicted mass transfer rate by ANN model 1 and model 2 for test data set

The criterion for selection of suitable ANN model is based on comparison between the relative error values for all the output data points estimated by using ANN model 1& 2 and is given in Table no. 5.

Table no.5: Relative error of predicted output values for mass transfer coefficient and mass transfer rate using ANN model 1 and ANN model-2 for training data.

Actual mass transfer coefficient	Predicted mass transfer coefficient Model1	Predicted mass transfer coefficient Model2	Mass transfer coefficient Relative Error model 1	Mass transfer coefficient Relative Error model 2	Actual mass transfer rate	Predicted mass transfer rate for Model 1	Predicted mass transfer rate for Model 2	Mass transfer rate for Relative Error for model 1	Mass transfer rate for Relative Error for model 2
3.2	3.225	3.177	-0.782	0.690	3	3.019	3.057	-0.647	-1.936
5.13	5.219	5.176	-1.745	-0.901	4.8	4.775	4.779	0.505	0.421
6.43	6.285	6.291	2.251	2.149	6	6.074	6.029	-1.247	-0.491
1.68	1.583	1.612	5.729	4.027	1.73	1.823	1.837	-5.398	-6.207
4.8	4.734	4.795	1.362	0.101	4.93	4.994	4.937	-1.306	-0.148
6.14	6.076	6.122	1.034	0.287	6.3	6.218	6.254	1.290	0.715
1.6	1.565	1.574	2.136	1.571	1.8	1.833	1.833	-1.835	-1.875
2.99	2.965	2.926	0.816	2.109	3.3	3.221	3.237	2.365	1.887
5.76	5.775	5.792	-0.261	-0.568	6.45	6.432	6.491	0.278	-0.636
1.58	1.547	1.556	2.0473	1.690	1.93	1.850	1.839	4.117	4.685
2.79	2.829	2.833	-1.130	-1.571	3.4	3.428	3.430	-0.827	-0.897
5.57	5.641	5.5478	-1.289	0.395	6.75	6.671	6.717	1.160	0.475
1.56	1.548	1.565	0.713	-0.347	1.73	1.870	1.824	-8.101	-5.437
3.74	3.810	3.739	-1.896	0.0037	4.13	4.020	4.095	2.645	0.824
4.49	4.672	4.573	-4.074	-1.850	4.95	4.875	4.933	1.510	0.332
1.48	1.547	1.544	-4.532	-4.346	1.8	1.895	1.842	-5.326	-2.339
2.39	2.414	2.420	-1.032	-1.289	2.9	2.866	2.824	1.146	2.598
4.46	4.497	4.411	-0.838	1.087	5.4	5.391	5.359	0.157	0.759
1.46	1.542	1.539	-5.648	-5.445	1.93	1.924	1.880	0.263	2.574
2.26	2.358	2.312	-4.338	-2.339	3	3.019	2.987	-0.663	0.411
4.31	4.332	4.284	-0.526	0.593	5.7	5.819	5.771	-2.089	-1.257
2.22	2.276	2.221	-2.524	-0.059	3.2	3.192	3.185	0.245	0.464
3.44	3.401	3.510	1.107	-2.058	4.93	4.935	4.869	-0.106	1.222
4.29	4.277	4.231	0.287	1.371	6.15	6.235	6.184	-1.386	-0.557
1.61	1.557	1.570	3.279	2.479	1.86	1.931	1.864	-3.843	-0.241
2.6	2.529	2.611	2.719	-0.438	3	3.046	2.986	-1.536	0.4379
5.21	5.049	5.157	3.081	0.999	6	6.107	6.001	-1.789	-0.018
1.52	1.553	1.554	-2.221	-2.291	1.93	1.956	1.912	-1.353	0.897
2.44	2.465	2.442	-1.050	-0.092	3.1	3.139	3.132	-1.264	-1.062
4.97	4.947	4.977	0.445	-0.142	6.3	6.336	6.323	-0.574	-0.375
2.38	2.393	2.276	-0.546	4.338	3.3	3.238	3.314	1.866	-0.453
3.66	3.689	3.707	-0.817	-1.309	5.06	5.104	5.087	-0.872	-0.548
4.78	4.808	4.800	-0.598	-0.427	6.6	6.478	6.540	1.839	0.899
1.46	1.538	1.569	-5.369	-7.482	2.2	2.008	2.151	8.701	2.182
3.56	3.604	3.494	-1.239	1.776	5.33	5.382	5.347	-0.980	-0.332
4.61	4.737	4.682	-2.765	-1.577	6.9	6.621	6.699	4.036	2.901

Fig no.9 & 10 show the graphs plotted between the relative error for the output parameters, mass transfer coefficient and mass transfer rate, estimated using ANN model 1 & ANN model 2 respectively for training data set. It is seen that there are deviations of the relative error from the mean value for the ANN models, 1 & 2. The range of relative error for the output parameter, mass transfer coefficient for ANN model 1 & ANN model 2 is 0-6 & 0-4 respectively. Similarly the range for the second output parameter, mass transfer rate for ANN model 1 & ANN model 2 is 0-8% & 0-4% respectively. As the relative error for ANN model 2 is lower for both the output parameters than estimated by ANN model 1, hence it can be said that the ANN model 2 is superior to the ANN model 1.

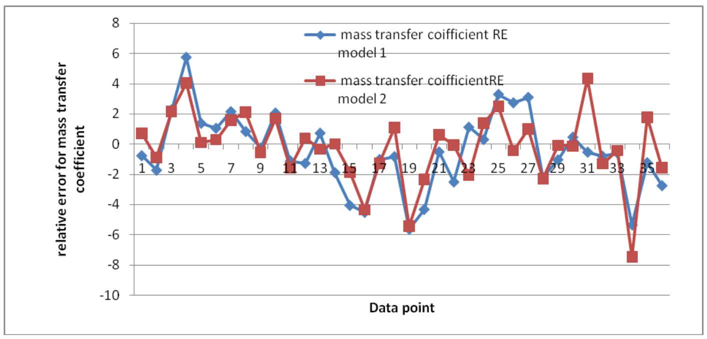

Figure no.9: Relative error of actual output and predicted output values for the mass transfer coefficient for training data

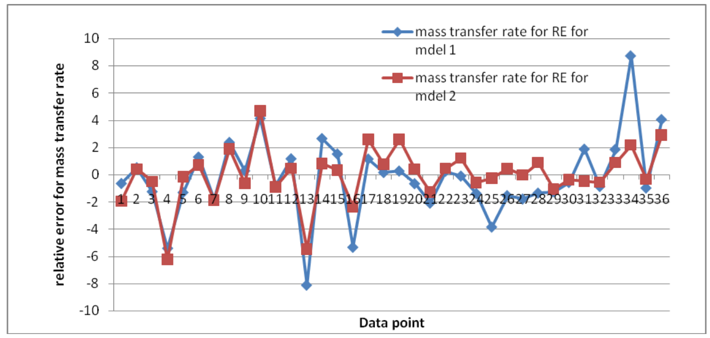

Figure no.10: Relative error of actual output and predicted output values for the mass transfer rate for training data

Similarly the relative error for all test data set points using models 1& 2 is calculated as given in Table 6.

Table no.6: Relative error of predicted output values of mass transfer coefficient and mass transfer rate for ANN model 1 and ANN model-2 for test data.

Actual mass transfer coefficient	Predicted mass transfer coefficient Model1	Predicted mass transfer coefficient Model2	Mass transfer coefficient Relative Error model 1	Mass transfer coefficient Relative Error model 2	Actual mass transfer rate	Predicted mass transfer rate for Model 1	Predicted mass transfer rate for Model 2	Mass transfer rate for Relative Error for model 1	Mass transfer rate for Relative Error for model 2
1.78	1.601	1.676	10.013	5.792	1.66	1.818	1.850	-9.569	-11.501
3.11	3.094	3.043	0.489	2.135	3.2	3.091	3.111	3.376	2.756
4.51	4.510	4.447	-0.010	1.385	5.06	5.296	5.166	-4.664	-2.105
4.28	4.482	4.229	-4.732	1.365	5.2	5.752	5.481	-10.62	-5.41
2.54	2.412	2.535	3.227	0.167	2.8	2.725	2.720	2.676	2.828
3.63	3.606	3.703	0.643	-2.020	4.4	4.238	4.343	3.673	1.290
3.52	3.467	3.617	1.554	-2.758	4.66	4.508	4.603	3.250	1.214
1.39	1.534	1.544	-10.400	-11.14	2	1.958	1.951	2.064	2.413
3.93	4.145	4.011	-5.488	-2.071	4.53	5.077	4.593	-12.09	-1.4
3.78	3.884	3.898	-2.756	-3.131	4.8	5.046	4.838	-5.142	-0.81
1.48	1.547	1.556	-4.569	-5.188	2.06	1.981	2.002	3.825	2.802
2.33	2.298	2.139	1.341	8.182	3.5	3.355	3.498	4.126	0.041

Fig no.11 & 12 show the graphs plotted between the relative error for the output parameters, mass transfer coefficient and mass transfer rate, for ANN model 1 & ANN model 2 respectively. It is seen that there are deviations of the percentage relative errors from the mean path of the ANN model 1 & 2. The range of relative errors for the output parameter, mass transfer coefficient for ANN model 1 & ANN model 2 is 0-10 & 0-6 respectively. Similarly the range for the second output parameter, mass transfer rate for ANN model 1 & ANN model 2 is 0-12 & 0-6 respectively. As the relative error for ANN model 2 is lower for both the output parameters than estimated by ANN model 1 for the training as well as test data set, hence it can be conclude that the ANN model 2 is superior to the ANN model 1 baring one point.

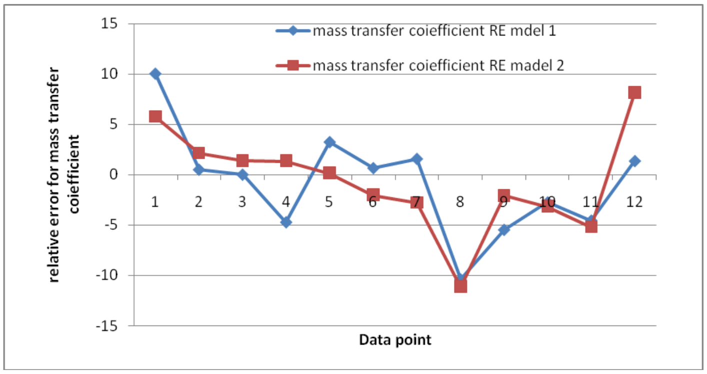

Figure no.11: Relative error of experimental output and predicted output values for the mass transfer coefficient.

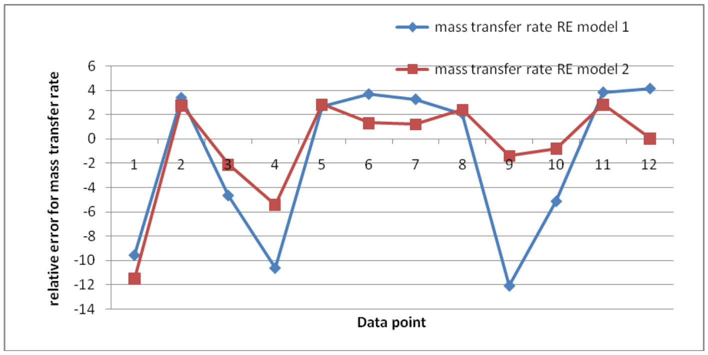

Figure no.12: Relative error of experimental output and predicted output values for the mass transfer rate.

VI. CONCLUSION

Artificial neural network models 1 & 2 are developed for modeling liquid-liquid extraction spray column, correlating mass transfer coefficient & mass transfer rate with flow-rate of extract phase , equilibrium concentration of acetic acid in aqueous phase & height of organic phase in column. The topology of the architecture was different for both the models. Based on results & discussions it can be concluded that both the models are successful in estimating the parameters but because of higher accuracy of estimation for both the training & test data sets ANN model 2 is more suitable. The work is demonstrative and the accuracy of estimation can be improved by altering the topology.

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