

Relationship between Strength Properties and Fiber Morphological Characteristics of *S. officinarum* – Part-1: Regression and Artificial Neural Networks Analysis

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Abstract: The impact of different pulp morphological properties on paper properties has been the subject of interest for paper makers. Relationships between the physical strength properties of *S. officinarum* pulp, like tensile index, tear index, burst index & double fold number, and the morphological characteristics of pulp fiber after at beating levels is developed in the present work. Multiple linear regression (MLR) and artificial neural networks (ANN) analysis are used to develop relationship models which can be useful to monitor and control quality of the paper products. The results have indicated that the MLR and ANN approaches can be successfully used to model the effects of beating on strength parameters of *S. officinarum* pulp.

Keywords: Multiple linear regression, Artificial neural network, *S. officinarum*, Morphological characteristics

1. Introduction

Paper is a highly heterogeneous composite material and its strength properties are dependent upon several factors like fiber properties, fiber distribution and fiber-fiber bonding. Moreover due to differences in the structure of every single fiber, even in the same pulp sample, the relationships between pulp fiber characteristics and paper properties show diverse complex relationships. The main limitation in prediction of paper properties is the lack of universal mathematical descriptions to describe relationship between properties and morphological features. The impact of different pulp morphological properties on paper properties has been the subject of interest for various investigators. Igmanson and Thode [1] studied the same, but they did not propose any final mathematical equations. A general mathematical relationship was introduced by Page [2, 3] to relate tensile strength with zero span tensile strength and other sheet parameters which are difficult to determine. Changes in the average fiber length occur mainly during the refining process and are considered as one of the main refining effects [4]. The significant influence of the average fiber length on paper strength properties was also confirmed by Clark [5], Paavilainen [6] and Olejnik [7]. At present none of the above investigations are able to predict and can be applied for the purpose of process control and decision making.

The complexity of the problem has initiated further research related to alternative solutions based on algorithms for advanced process modeling, control and optimization. Multiple linear regression (MLR) and artificial neural

networks (ANN) are the promising techniques and can be used to develop models of relationships between the morphological characteristics which can be then used to control the process of refining and ensure quality of the product. Among the significant studies of MLR modeling in pulp and paper industry, Jahan and Rawshan [10],developed regression models for prediction of the effect of jute pulp addition and the beating degree on paper properties. Another method was proposed by Chagaev and Zou [11] in which they introduced the pulp quality index and fiber development index based on the content ratio of fines to coarse fibers to monitor strength development during mechanical pulp refining. Efforts have been made to explore the relationship between chemical and physical properties of the pulp fiber and their inherent paper making strength properties by various researchers [12-19].

Possibility of application of ANN in the paper industry has also been reported in various articles [20-25]. Ciesielski and Olejnik [26] developed a predictive, neural network based model which enables the prediction of paper properties based on factors related to the most important refining effects, such as the fiber and pulp WRV, average fiber length and fine content. Similar work has been reported by Nieminen et al. [27] using data from a pilot plant paper machine. Edwards et al.[28] reported the application of neural network techniques for the prediction of paper curl and the techniques was found to be applicable to industry.

Literature studies have shown that a no work is reported on relationship of morphological characteristics and strength properties of paper made from *S. officinarum* pulp. Therefore

development of models for paper strength properties based on influence of morphological characteristics for *S. officinarum* pulp will be helpful for the paper industry to optimize and control the quality of paper. In present article application of multiple linear regression and artificial neural networks is presented for development of appropriate models to predict paper strength properties of *S. officinarum* pulp subjected to different beating levels in a laboratory PFI mill.

2. Experimental

Materials and Methods

S. officinarum, collected from a sugar mill located in Haryana, India, was subjected to mechanical treatment i.e. dry and wet depithing followed by intensive screening to remove most of the non-fibrous cells. Dry depithing was done in dry depither (Bramco, BD 101, India). Further, the depithed bagasse was disintegrated in hydropulper (wet depithing) to remove rest of the pith cells at 2.5% consistency and screened in Wevrek vibratory screen of mesh size (-)150 as per TAPPI UM 03.

Soda-anthraquinone (AQ) pulping of the depithed bagasse was carried out in electrically heated laboratory rotary digester (Make-Weverk). The cooking conditions maintained were; Top temperature 160 °C, time 60 min, active alkali charge 12% (as Na₂O), liquor to raw material ratio 4.5:1 and AQ 0.1% on o.d. weight of raw material.

Unbleached soda-AQ pulp was bleached using XOCEH1H2 bleaching sequence, where „X” stands for xylanase stage, „O” for oxygen bleaching stage, „C” for chlorination, „E” for alkaline extraction, „H1” for hypochlorite 1st stage and „H2” for hypochlorite 2nd stage.

The bleached pulp of *S. officinarum* was beaten in a PFI mill as per TAPPI T 248 sp-00 “Laboratory beating of pulp [PFI mill method]”, at different beating levels. Each pulp sample was analyzed for morphological characterization using Morphi laboratory fiber analyser. The morphological characteristics evaluated were fiber length, fiber width, coarseness, kink angle, kinked fibers, curl rate in length of micro fibril, broken ends, fine elements (% in length) and % fines (% of area).

Laboratory handsheets of 60 g/m² were prepared on a British sheet former using TAPPI T 205cm-99 “Forming hand sheet for physical test of pulp”. Handsheets were pressed, air-dried under atmospheric conditions, preconditioned at 27±2 °C at a relative humidity of 65±2% and evaluated for various physical strength properties, such as tear index (TAPPI T 414 om-98 “Internal tearing resistance of paper [Elmendorf-type method]”), tensile index (TAPPI 494 om-01 “Tensile properties of paper and paperboard using constant rate of elongation apparatus”), burst index (TAPPI T 403 om-97 “Bursting strength of paper”), double fold (TAPPI T 423 cm-98 “Folding endurance of paper”).

MLR and ANN Modeling methods

Multiple linear regression (MLR) and feed forward artificial neural networks (ANN) were used to predict the mechanical properties of handsheets made from *S. officinarum* pulps.

Statistical software SPSS 16.0 was used for MLR analysis. Physical strength properties of paper viz., tensile index, tear index, burst index and double fold were used as dependent variables and the morphological parameters of the pulp at different level of beating as independent variables. Only statistically significant linear regression equations (ANOVA, p-value ≤ 0.5%) are reported in the present work. The percentage deviation between the experimental and calculated values from the multiple regression equations for tensile index, tear index, double fold and burst index, were used to validate the most significant MLR models.

Artificial neural networks, has emerged as a promising solution due to evaluation of non-linear relationship between fiber characteristics and physical and mechanical properties of paper. These models perform a non-linear transformation of input data to approximate output data, learning from experimental data examples and exhibiting some ability for generalization beyond training data. The most common artificial neural network is the multilayer feed forward artificial neural network where the nodes are grouped into three types of layers, i.e. input, hidden and output layers. Input data are provided to the nodes in the input layer which are then transferred to the subsequent layers. Cybenko [29] has shown that a one hidden layer ANN is enough to approximate any function, if presenting enough hidden nodes. The topology of the network, along with the neuron processing function, determines the accuracy and degree of representation of the model developed to correctly represent the system behavior.

The MATLAB Neural Network Toolbox was used for the configuration of the models. The data were randomly divided into three sets, training, validation and testing, for tensile index, tear index, double fold and burst index. 70% samples were used for the ANN training process for each of the outputs, i.e., tensile strength, tear index, double fold and burst index, while the remaining 30% samples were equally divided for validation and testing processes. The percentage error between the predicted values from the experimental samples for tensile index, tear index, double fold and burst index, were used as the performance criteria of the ANN models. The mean absolute error (MAE), the mean absolute percentage error (MAPE), the root mean square error (RMSE), and correlation coefficient (R^2) were used to evaluate the prediction performance of the models. The models yielding the best results for tensile index tear index, burst index and double fold were considered as the prediction models. [30].

One layer feed-forward network with sigmoid hidden neurons and linear output neurons were used as the activation functions to fit multi-dimensional mapping problems. The transfer function used for one layer feed forward network was “PURELIN”. This was helpful to compare the one layer

ANN results using PURELIN transfer function with the Multiple Linear Regression analysis. The Levenberg-Marquardt back propagation algorithm was chosen as the training algorithm in all cases.

Morphological characteristics of *S. officinarum* pulp fibers at different beating levels were used as input variables and tensile index, tear index, double fold & burst index as output variables in the models.

3. Results & Discussion

Multiple Linear Regression (MLR) Analysis between Strength Properties and Morphological Characteristics of *S. officinarum*

Beating of pulp fibers is an important paper making process operation. During beating the mechanical stresses imposed on pulp fibers, significantly affect the morphological characteristics of the fibers and thus influence the mechanical

strength properties of paper sheets. It is reported that after removal of primary wall of fibers (first beating effect), the shrinkage in length of fibers is ~20%, whereas the width is reported to increase by ~65% [31]. The fiber swelling enhances the fiber flexibility and area for hydrogen bonding increases. Therefore, all the mechanical strength properties depending upon hydrogen bonding improve, except tear strength. Tear strength of paper depends on the fiber's behavior in the rupture zone and the necessary work that has to be done to pull the fibers loose, depends on the length of the fibers as well as the inter fiber bond strength. During tear the fracture propagates across the sample, therefore due to weak hydrogen bonding compared to strength of the fibers at low level of beating, the fibers tend to be pulled out intact. At higher levels of beating, the inter fiber bond strength will be higher, therefore fibers start to break instead of being pulled out intact.

Table 1: Morphological characteristics of *S. officinarum* pulp fibers at different beating levels

Parameters	Values						
CSF, ml	595	542	510	455	390	338	305
Weighted fiber length, mm	0.791	0.784	0.778	0.774	0.763	0.755	0.742
Fiber width, (μm)	24.5	24.92	25.1	25.38	25.6	25.9	25.95
Coarseness, (mg/m)	0.0646	0.061	0.0574	0.0532	0.0448	0.0424	0.0418
Kink angle, ($^{\circ}$)	119	120	121	122	123	123	124
Kinked Fibers, (%)	40.3	39.2	38.5	37.8	34.2	32.3	32
Curl, (%)	12.7	12.6	12.5	12.4	12.3	12.1	12
Rate in length of Macro fibrils, (%)	0.744	0.884	0.983	1.126	1.182	1.304	1.325
Broken Ends, (%)	33.42	33.58	33.76	33.85	34.02	34.11	34.25
Fine elements, (% in length)	46.7	46.9	47.1	47.6	48.1	48.4	49
% fines, (%area)	17.93	18.04	18.14	18.23	18.35	18.52	18.94

Table 1: *contd...*

Parameters	Values					
CSF, ml	286	270	244	224	212	190
Weighted fiber length, mm	0.739	0.73	0.725	0.721	0.719	0.718
Fiber width, (μm)	25.98	25.99	26	26.08	26.06	26.05
Coarseness, (mg/m)	0.0412	0.040	0.0406	0.0404	0.0404	0.0403
Kink angle, ($^{\circ}$)	125	126	126	127	128	130
Kinked Fibers, (%)	31.7	31.3	31.1	30.7	30.4	30.1
Curl, (%)	11.9	11.8	11.7	11.4	11.2	10.9
Rate in length of Macro fibrils, (%)	1.352	1.408	1.449	1.461	1.473	1.482
Broken Ends, (%)	34.42	34.61	34.76	34.05	35.16	35.23
Fine elements, (% in length)	49.7	50.3	50.4	50.1	51.2	51.5
% fines, (%area)	19.87	20.21	20.65	20.98	21.37	21.54

Table 2: The measured values of strength parameters for *S. officinarum* pulp handsheets at different beating levels

CSF, ml	Tensile index, Nm/g	Tear index, mNm ² /g	Burst index, kPam ² /g	Double fold
595	24.17±1.22	3.52±0.42	1.12±0.22	6±0.29
542	29.28±1.36	3.58±0.21	1.34±0.25	7±0.27
510	36.46±1.21	3.64±0.25	1.48±0.27	8±0.56
455	42.27±1.32	3.97±0.31	1.87±0.29	9±0.38
390	50.42±1.46	4.26±0.29	2.94±0.16	12±0.59
338	56.41±1.20	4.82±0.27	3.62±0.43	14±1.21
305	60.56±1.58	4.78±0.45	4.11±0.45	15±1.19
286	62.20±1.67	4.53±0.41	4.26±0.38	16±1.52
270	64.35±1.42	4.29±0.27	4.42±0.34	18±1.25
244	67.24±1.29	3.96±0.54	4.57±0.28	20±1.17

224	66.97±1.41	3.72±0.38	4.51±0.30	18±1.16
212	66.12±1.29	3.43±0.47	4.45±0.23	13±0.96
190	65.26±1.78	3.18±0.35	4.41±0.39	9±0.84

± refers standard deviation

The MLR analysis of relationship between various physical strength properties, like tear index, tensile index, burst index and double fold (Table 2) and the change in morphological characteristics of the fibers of *S. officinarum* after different beating levels (Table 1) has also shown similar behavior. The results of MLR analysis showing correlation of the significant morphological parameters with physical strength properties are presented in Table -3.

Results of stepwise MLR analysis presented in Table-3 reveal that fiber length, fiber width, coarseness and curl significantly affect the tensile strength of hand sheets made from *S. officinarum*. The most dominating independent variables are fiber length and curl which account for 98.6% and 98.5%

respectively. Fiber width and coarseness account for 95.6% and 81.8% of the variations respectively. The multiple regression analysis involving these variables accounted for 99.7% of the total variation.

Table 3: MLR analysis of relationship between tensile index, tear index, burst index and double fold numbers and significant morphological characteristics of *S. officinarum* pulp fibers

Dep. Var*	Predictors	Coeffi-cient	Sig. *	Ind. R ² *	Mult R ² *	
Tensile index, Nm/g	Constant	89.518	.397	-	0.997	
	Fiber length, mm (X ₂)	-376.739	.049	0.986		
	Fiber width, μm (X ₃)	7.568	.000	0.956		
	Coarseness, mg/m (X ₄)	-550.014	.000	0.818		
	Curl, % (X ₇)	6.483	.017	0.985		
Regression model: Tensile index (Nm/g) = -376.739 X₂ + 7.568 X₃ - 550.014 X₄ + 6.483 X₇ + 89.51						
Tear index, mNm ² /g	Non-significant correlations among dependent and independent variables					
Burst index, kPam ² /g	Constant	68.739	.000	-	0.990	
	Fiber length, mm (X ₂)	-54.180	.001	0.957		
	Coarseness, mg/m (X ₄)	-118.640	.000	0.970		
	Kink angle, degree (X ₅)	-0.127	.004	0.839		
	Percentage in length of Macrofibrils, % (X ₈)	-2.837	.047	0.966		
Regression model: Burst index (kPam²/g) = - 54.180 X₂ - 118.640 X₄ - 0.127 X₅ - 2.837 X₈ + 68.739						
Double fold, number	Constant	-178.853	.010		0.965	
	CSF, mL (X ₁)	-0.074	.000	0.344		
	Curl, % (X ₇)	19.679	.000	0.216		
	Broken ends, %(X ₉)	-2.873	.000	0.547		
	Fine elements, % in area (X ₁₁)	4.132	.022	0.204		
Regression model: Double fold (number) = -0.074 X₁ + 19.679 X₇ - 2.873 X₉ + 4.132 X₁₁ - 178.853						

*dependent Variable, significance, Individual R², Multiple R²

However, the stepwise multiple linear regression analysis between tear index and various morphological characteristics of *S. officinarum* pulp fibers resulted in non-significant correlation among dependent and independent variables. The significance levels of all the independent variables were found to be greater than 0.05 and therefore no regression model could be suggested.

The tear index values of *S. officinarum* pulp sheets after beating to different beating levels indicate non-linear relationship between tear index and morphological characteristics. It increases from 3.5 to 4.82 mNm²/g on beating from 595 to 338 CSF (mL) and on further beating from 338 mL CSF to 173 mL CSF, it drops from 4.82 to 2.49 mNm²/g. The non-linear relationship between tear index and morphological characteristics of *S. officinarum* therefore could not be established using MLR analysis.

MLR analysis between burst index and morphological characteristics of pulp fibers revealed that fiber length, coarseness, kink angle and percentage in length of macrofibrils significantly affect the burst index of handsheets made from *S. officinarum* pulp. Coarseness and percentage in length of macrofibrils are most dominating individual variables and account for 97.0% and 96.6% respectively towards burst index variation. Fiber length and kink angle account for 95.7% and 83.9 % variation individually. The multiple regression analysis involving combined effect of these variables accounted for 99.0% of the total variation.

Relationship between double fold and morphological characteristics of pulp fibers after beating of pulp upto different levels revealed that CSF, curl, broken ends and fine elements (% in area) significantly affect the double fold number of *S. officinarum* pulp handsheets.

Broken ends account for 54.7 % variation. The other factors affecting double fold are CSF, Curl and Fines elements (% in area). The multiple regression analysis involving combined effect of these variables was found to account for 96.5 % of the total variation.

The regression models of relationship between tensile index, burst index & double fold (dependent variables) and various morphological characteristics (independent variables) were validated using experimental data limits. The percent deviation between experimental and the calculated values of tensile index were found to be within the acceptable limits. However in case of burst index and double fold the percent deviation between experimental and the calculated values were observed to be on higher side (Table 4). This is due to non linear relationship between CSF values and the double fold values in the higher beating levels.

Table 4: Percentage Deviation between experimental and the calculated values of strength properties

S. No.	CSF, mL	% Deviation between experimental and the calculated values of strength properties.		
		Tensile index, Nm/g	Burst index, kPam ² /g	Double fold, number
1	595	1.78	11.16	14.82
2	390	0.97	5.78	3.51
3	270	0.23	4.03	3.04
4	173	0.85	1.80	6.23

Artificial Neural Network analysis of Strength Properties and Morphological Characteristics of *S. officinarum*

The morphological characteristics of *S. officinarum* pulps, beaten to different freeness levels (Table 1) were used for the ANN testing, training and validation process for hand sheet strength parameters, as input variables. The output variables in the models were the measured values of tensile index, tear index, double fold and burst index for different pulp freeness levels of pulps (Table 2).

Figure-1 shows a typical Neural Network Performance plot for training, validation and test data for tensile properties of *S. officinarum* handsheets data as dependent and morphological parameters as independent functions.

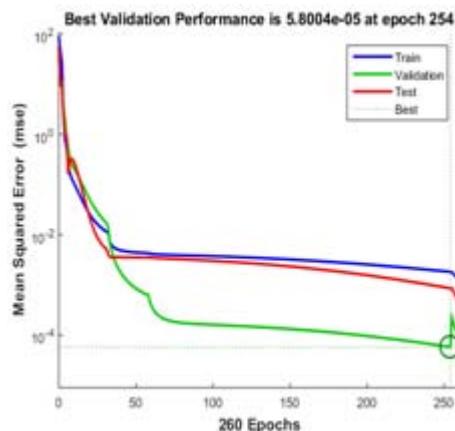


Figure 1: A typical Neural Network Performance plot for training, validation and test data

The percentage error between the predicted values from the experimental samples for tensile index, tear index, double fold and burst index was used as the performance criteria of the ANN models. The predicted values and percentage errors observed in tensile index tear index, double fold and burst index for hand sheets made from *S. officinarum* pulps are shown in Table 4.

Table 4: Predicted values and percentage errors of strength properties of *S. officinarum* handsheets using one layer linear ANN networks

CSF	Tensile Index		Tear Index		Burst Index		Double fold	
	P*	E*	P*	E*	P*	E*	P*	E*
595	24.17	-1.29	2.49	1.03	1.17	-0.05	2	4.49
542	29.28	0.75	3.62	-0.04	1.28	0.05	1	5.85
510	36.46	-0.14	2.49	1.15	1.49	-0.01	1	6.87
455	42.27	-0.06	2.49	1.48	1.87	0.00	1	7.88
390	50.42	0.11	4.82	-0.56	2.93	0.01	6	6.21
338	56.41	-0.14	4.82	0.00	3.62	-0.01	7	7.44
305	60.56	0.03	4.82	-0.04	4.10	0.00	10	5.28
286	62.2	-0.46	4.82	-0.29	4.27	-0.02	12	4.12
270	64.35	0.09	4.24	0.05	4.41	0.00	11	6.55
244	67.24	0.38	3.98	-0.02	4.54	0.02	5	14.93
224	66.97	0.09	2.49	1.23	4.50	0.00	5	12.78
212	66.12	0.41	2.49	0.94	4.43	0.012	7	5.69
190	65.26	0.38	2.49	0.69	4.37	0.037	5	3.53
173	64.44	-0.52	2.49	0.00	4.35	-0.02	2	4.77

*P and E denote predicted values and error in % respectively

Results show that while comparing predicted values to measured values, in most of the cases the neural network prediction is very close to the measured values, except tear index and double fold values. This is due to the errors caused by the material, the measurements and process parameters [30].

Performance criteria values used to assess the performance of the proposed prediction models are given in Table 5. The prediction values were clearly determined with very low percentage errors. The low level of errors is satisfactory for predicting the strength properties of the hand sheets. This also demonstrates that the networks effectively give accurate results.

Table 5: Performance criteria used for predicting various strength properties of *S. officinarum* hand sheets using one layer linear ANN networks

Performance criteria	Tensile Index			Tear Index		
	1*	2*	3*	1*	2*	3*
MAE	0.000	0.000	0.000	0.499	0.180	0.379
MAPE	0.000	0.000	0.000	0.434	0.746	1.623
RMSE	0.000	0.000	0.000	2.593	0.441	0.929
R2	1.000	1.000	1.000	0.985	0.997	0.987

*1= Training, 2= validation, 3= Testing

Performance criteria	Burst Index			Double fold		
	1*	2*	3*	1*	2*	3*
MAE	0.004	-0.001	-0.006	7.926	5.500	7.333
MAPE	0.003	-0.008	-0.029	2.125	8.088	9.778
RMSE	0.018	0.003	0.015	41.18	13.472	17.963
R2	1.000	1.000	1.000	0.661	0.718	0.603

*1= Training, 2= validation, 3= Testing

Regression analysis between the predicted values and the measured values is generally used to assess the validity of the networks and their accuracy. Figures 2 to 5 show the relationship between the measured values and predicted values for training data, validation data, testing data and all data in predicting tensile index, tear index, double fold and burst index, respectively.

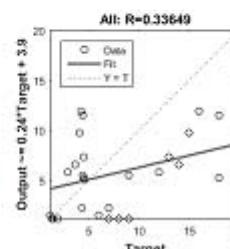
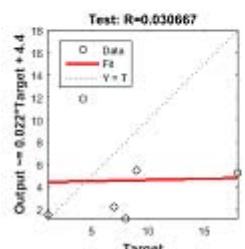
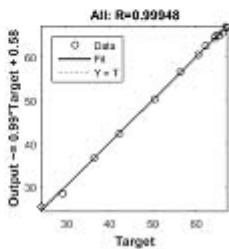
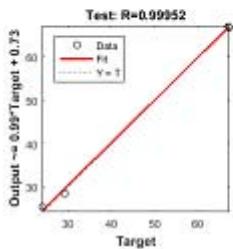
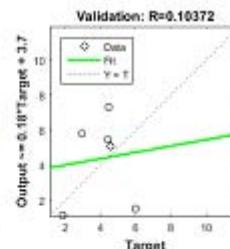
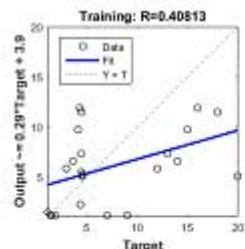
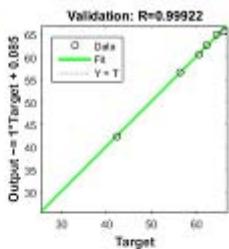
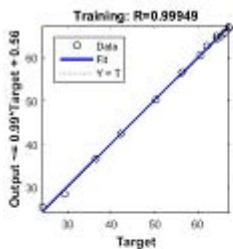


Figure 2: Relationship between measured results and predicted results for tensile index of *S. officinarum* handsheets using one layer linear ANN networks.

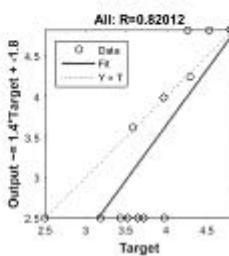
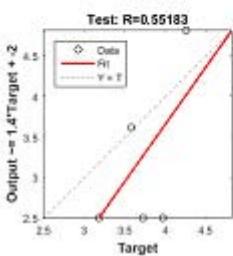
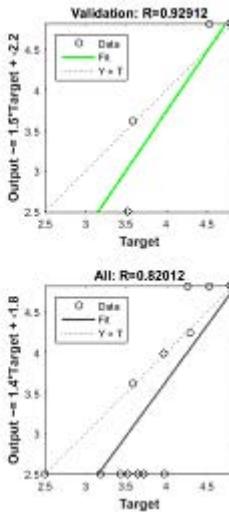
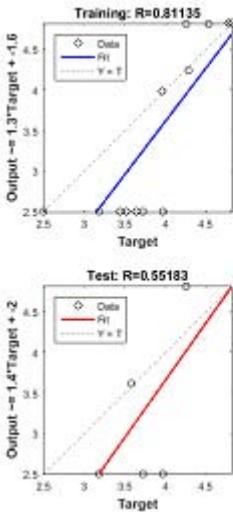


Figure 3: Relationship between measured results and predicted results for Tear Index of *S. officinarum* handsheets using one layer linear ANN networks.

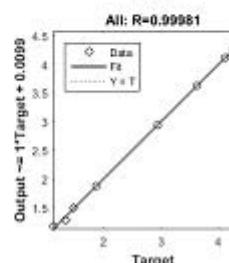
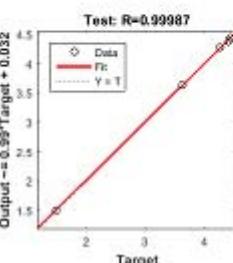
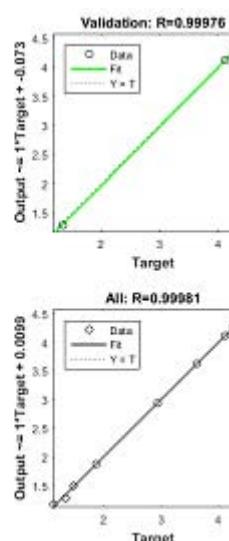
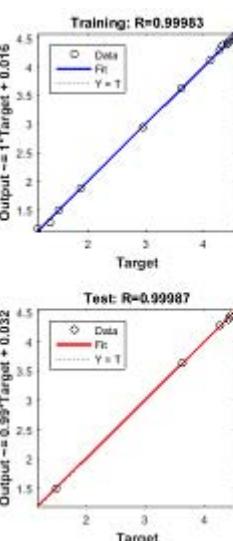


Figure 4: Relationship between measured results and predicted results for Burst Index of *S. officinarum* handsheets using one layer linear ANN networks.

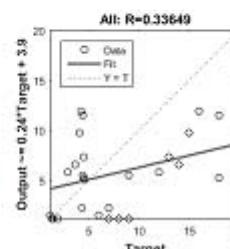
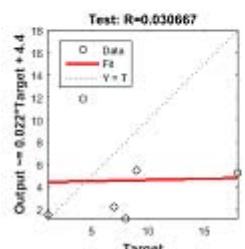
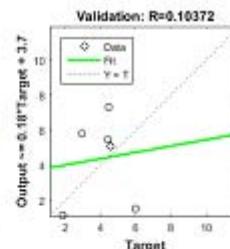
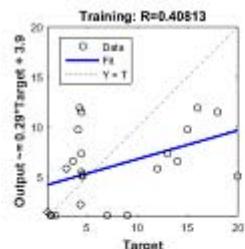


Figure 5: Relationship between measured results and predicted results for Double fold number of *S. officinarum* handsheets using one layer linear ANN networks.

In Figures 2 - 5, the predicted values are plotted against the measured values as open circles. The best linear relationship is shown with a dashed line. In addition, the perfect linear relationship between measured values and the predicted values in predicting tensile index and burst index is indicated by a solid line.

The accuracy of the prediction models for tensile index of handsheets made out of *S. officinarum* pulp is proved by the increasing correlation coefficient (R^2) values. As R^2 approaches 1, prediction accuracy increases. Analysis of the measured and predictive results of tensile index, tear index, burst index and double fold for *S. officinarum* handsheets using one layer ANN network with linear transfer function reveals that the predicted values are very close to the measured values for all parameters, except in case of tear index and double fold. This strengthens the reliability of the ANN models as they successfully predict correlation of the strength properties with morphological parameters without time consuming and costly comprehensive experimental investigations. The ANN results also compliment the MLR analysis results as the tear and double fold values between measured results and predicted results do not show co-linearity.

4. Conclusion

The predicted results of relationship between physical strength properties and morphological characteristics using MLR and ANN analysis are highly satisfactory in terms of explanatory characteristics and validity of the models. The results indicate that the MLR and ANN approach can be successfully used to model the effects of *S. officinarum* pulp beating degree on strength parameters. This study therefore permits a preliminary decision to be made concerning usability under conditions in which the strength properties of paper are important. The MLR and ANN models can be used to design tailor-made products meeting specific requirements by altering the morphological characteristics of the pulp fibers. This approach would save time, reduce the

consumption of experimental materials and lower design costs for paper industry.

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