ARTIFICIAL NEURAL NETWORK MODELING AND OPTIMIZATION OF SHAMPOO FORMULATIONS

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INTRODUCTION

The artificial neural network (ANN) method for data analysis is very popular and has been used in many areas including tablet formulations, controlled release drug delivery studies, and also in cosmetic science. In this study, we designed and tested shampoo formulations then optimized according to their viscosity and foam properties. Our aim was to show the usefulness of artificial neural network methodology in developing and optimizing shampoo formulations.

MATERIALS AND METHODS

Materials

Texapon (70 %) [SLES (Sodium lauril ether sulfhate)], Betaine (45 %) (Cocoamidpropyl betaine) were used as primary surfactant, and NaCl was used to adjust viscosity. An ANN software (STATISTICA, Neural Networks, Release 4.0, StatSoft, USA) was used for modeling and optimization.

Methods

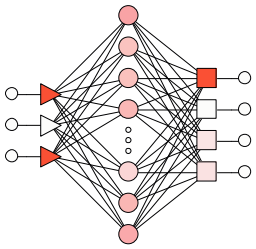
Thirty three shampoo formulations were prepared and each of them had SLES between 6 - 12 %, betaine 1,5 - 7,5 %, and NaCl 1 – 7 %. SLES and betaine were added to water then NaCl solution was added to formulations. Each formulation was prepared as 200 g.

Factors and measured characteristics

SLES, betaine and NaCl concentrations were used as the independent variables. Viscosity, pH, dry foam and standard foam were defined as the dependent variables. To measure the foam capacity, a 0,5 g sample from each formulation was diluted with 50 ml (40ºC) distilled water and stirred on a magnetic stirrer then immediately was poured into a graduated cylinder and 20 constant shaking applied in that cylinder. We noted the first and the 5th-minute foam capacities. For modeling purposes, out of 32 experiments 22 were reserved for network *training*, 6 for *test*, and 5 for model *verification*.

RESULTS AND DISCUSSION

After testing 33 formulations, when the other parameters were constant, only NaCl concentration was evaluated. It was observed that between 3 – 5 %, viscosity was very high and if we increased the concentration to 7 %, it decreased again. If we examine SLES and betaine together, the viscosity increases with their concentration. Increasing NaCl concentration also increased the foam capacity. The best models were constructed using the ***radial basis function*** (RBF). The constrains for the optimum formulation were : A viscosity under 10.000 cps, dry foam and standard foam with the maximum values. There were many combinations which were satisfactory. One of them was : SLES 12 %, betaine 1,5 %, NaCl 7 % that resulted in a pH 5,81, viscosity of 6500 cps, dry foam of 194 ml and a standard foam of 158 ml. Overall, the ANN was found to be an excellent tool for data analysis.

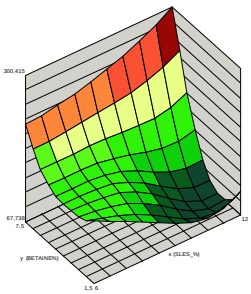


A typical network architecture for RBF (3 – 13 - 4)

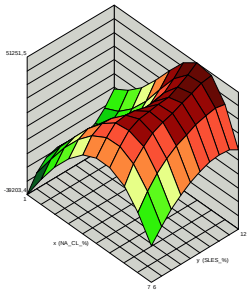
Dependent variables : pH, Viscosity, Dry Foam, Std Foam

Network Type:	RBF (3-13-4)
Number of inputs:	3 (1,2,3)
Training-test- verification	22-6-5
Network performance	**Very Good**
Regression ratio	0.106446
Correlation	0.996370
Error	0.04082
RMS Error	
Training	0.03585
Verification	0.04082
Test	0.7417

Inputs: SLES, Betaine
Output: Dry foam



Inputs: NaCl, SLES
Output: Viscosity



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2. Turkoglu, M., Aydin, I., Murray, M., and Sakr A, Modeling of a roller-compaction process using neural networks and genetic algorithms. Eur. J. Pharm. Biopharm. 48(3) 239-245 (1999)