Comparative Evaluation of Artificial Neural Networks and Data Analysis in Predicting Liposomes Size in a Periodic Disturbance Micromixer

Ixchel Ocampo[1], Rubén R. López[2,3], Vahé Nerguizian[3], Ion Stiharu[4*], Sergio Camacho-León1[1]

1 School of Engineering and Sciences, Tecnológico de Monterrey, Av. Eugenio Garza Sada 2501 Sur, Monterrey 64849, N.L., México; A00800468@itesm.mx (I.O.); sergio.camacho@tec.mx (S.C.-L.)
2 Departments of Oncology & Pathology, McGill University, Cancer Research Program, MUHC-RI, 1001 Décarie, Montreal, QC, H4A 3J1, Canada; ruben.lopezsalazar@mail.mcgill.ca (R.L.S.)
3 Department of Electrical Engineering, École de technologie supérieure, 1100 Notre Dame West, Montreal, QC, H3C 1K3, Canada; vahe.nerguizian@etsmtl.ca (V.N.)
4 Department of Mechanical and Industrial Engineering, Concordia University, 1455 de Maisonneuve Blvd. West, Montreal, QC, H3G 1M8, Canada; * Correspondence: ion.stiharu@concordia.ca; Tel.: +1-514-848-2424 (ext. 3152)

Abstract

Artificial Neural Network (ANN) and Data Analysis (DA) are powerful tools used for supporting decision-making. They have been employed in diverse fields and one of them is nanotechnology; for example, in predicting particles size. Liposomes are nanoparticles used in different biomedical applications that can be produced in Dean Forces-based Periodic Disturbance Micromixers (PDM). In this work, ANN and DA techniques are used to build a liposome size (LZ) prediction model by using the most relevant variables in a PDM, i.e. Flow Rate Radio (FRR) and Total Flow Rate (TFR). The ANN was designed in MATLAB and fed data from 60 experiments, which were 70% training, 15% validation and 15% testing. For DA, regression analysis was used. The model was evaluated, it showed 98.147% of regression number for training and 97.247% in total data comparing with 78.89% regression number obtained by DA. These results demonstrate that liposomes size can be better predicted by ANN with just FRR and TFR as inputs, compared with DA techniques when the temperature, solvents, and concentrations are kept constants.

Introduction

DA tools are commonly used for size prediction of liposomes fabrication by micromixers. These tools have made possible finding a ratio between the FRR and TFR parameters and the average size of the obtained liposome. However, the performance of these techniques are limited. The implementation of an ANN could allow the development of more accurate models [1]. Comparative studies of both techniques are required to determine the one with the best performance.

EXPERIMENTAL

The liposome size prediction model based on DA techniques was previously supported in "Surface Response Based Modeling of Liposome Characteristics in a Periodic Disturbance Mixer" [2] and it was given by the following equation:

$$Z_{avarage} = 236.3 - 26.95FRR - 4.437TFR + 1.573(FRR)^2$$

On the other hand, the ANN was a two-layer feed-forward network with sigmoid hidden neurons and linear output neurons, known as curve fitting [3], it consisted of 2 input (FRR, TFR) and 1 output (LZ) variables with 60 samples. 70% of data were used for training, 15% for validation and finally 15% for testing. This ANN was programmed by MATLAB, using nnstart toolbox.

Table 1. *Validation table is conformed by FRR and TFR selected to verify the performance of the model's vs the real measured value.*

	FRR (ml/h)	TFR (ml/h)	REAL (nm)	ANN (nm)	DA (nm)
1	10.40	5.20	120.2	121.021	103.083
2	12.02	10.50	73.8	74.9883	92.990
3	6.50	10.50	77.24	78.9807	80.995
4	5.00	18.00	64.7	64.2887	61.009
5	3.30	3.10	199.1	199.084	168.747

RESULTS AND DISCUSSION

The ANN showed 98.147% of regression number for training and 97.247% in total DA data, compared with 78.89% regression number obtained by DA [4].

The Table 1 shows the values used to validate the model's efficiency, where 5 selected FRR and TFR (ml/h) were tested with the 2 models. Figure 1 shows the LZ obtained with ANN, DA models and the real measured value. These results demonstrate that liposomes size is better predicted by ANN, compared with data analysis techniques with the same input variables [FRR, TFRR] when the temperature, solvents, micromixer, and concentrations are kept constants.

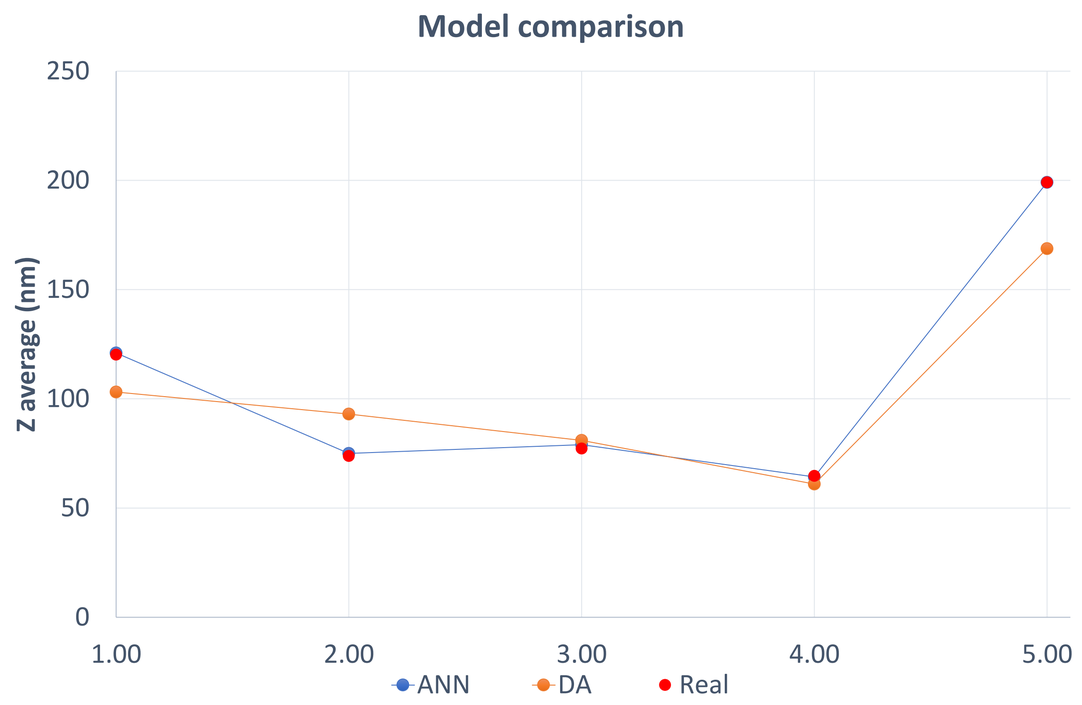

Figure 1. Model comparison graph: *The graphic shows Liposomes size according to the prediction models, blue line is ANN , orange line is DA and red points are the real measured values.*

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Contact

Dr. Ion Stiharu
Department of Mechanical and Industrial Engineering, Concordia University
ion.stiharu@concordia.ca
+1-514-848-2424 (ext. 3152)

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