EngOpt2018 - 6th International Conference on Engineering Optimization
Instituto Superior Técnico, Lisbon Portugal • 17-19 September, 2018
Editors: H.C. Rodrigues, J. Herskovits, C.M. Mota Soares, et al.

Abstract ID 1121

OPTIMIZATION OF POLYACRYLAMIDE BASED MULTICOMPONENT HYDROGELS SYNTHESIS USING A NEURO-EVOLUTIONARY STRATEGY

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Keywords: Differential Evolution,Artificial Neural Networks,Process optimization,Multicomponent hydrogels

Abstract: In this work, the synthesis of polyacrylamide based multicomponent hydrogels is modelled using a neuro-evolutive technique which combines Differential Evolution (DE) algoritm and Artificial Neural Networks (ANNs). The neural model is developed in an optimal form applying the DE procedure, meaning the optimization of the weights, biases and architecture (number of hidden layers, neurons in each hidden layer and their activation function). The data set used in modelling action contains experimental data obtained in our laboratory. Based on the neural model, the process is further optimized with DE algorithm in order to determine the optimum conditions of the synthesis (time, temperature, monomer concentration, initiator, crosslinking agent, inclusion polymer, and type of the polymer added) leading to the maximization of the reaction yield. In order to improve the performance of the DE algorithm, different research directions were followed in this work: i) the use of self-adaptability to automatically determine the optimum values for the control parameters of the optimization algorithm; ii) the modification at step level of DE (chaotic maps for the initial population and a modified mutation strategy that has a higher probability of providing better individuals); iii) hybridization with Backpropagation and/or Local Search algorithm for the best solution found so far. The simulation results indicated that the best model, as individual multilayer perceptron, has a (7:10:1) structure, where 7 indicates the number of inputs (process parameters), 10 the number of neurons in the hidden layer and 1 the number of outputs (reaction yield). The obtained errors are: 7.54% average absolute error (AARE), 0.96 correlation (COREL) and 0.36 mean squared error (MSE) for training and 9.23% AARE, 0.967 COREL, 0.722 MSE for testing. Even this model can be considered satisfactory, a stack neural network was developed, composed from three simple individual networks, also applying the optimization with DE algorithm. In this way, the errors were reduced with more than 4%. The optimization of the process, using the stack neural model, provides the working conditions that lead to a reaction yield of 96%. Some restrictions were imposed to the reaction conditions for reducing the material and time consumption. From the points of view of result accuracy and method accessibility, the optimization method based on ANN and DE, applied both to model and process, can be considered appropriate for the approach system, capturing in an efficient way the dynamic of the process.