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Hybrid neural networks as tools for predicting the phase behavior of colloidal systems

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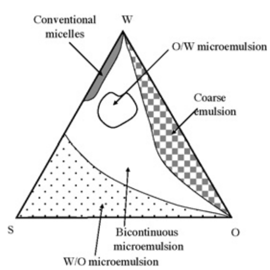
HIGHLIGHTS

- ► Formulating a stable microemulsion is a time consuming, empirically based process.
- ► Using predictive models can reduce the time and cost of formulation development.
- ► Surfactant (or surfactant/co-surfactant), oil and water systems were investigated.
- ► Hybrid neural networks were used to model the phase behaviour of these systems.
- ► The best performing network in our study predicted 81.6% of the data correctly.

GRAPHICAL ABSTRACT



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ABSTRACT

The aim of this study was to use hybrid NNs with categorical (discrete) outputs, rather than encoded binary outputs to model phase behaviour of quaternary colloidal systems, and to predict microemulsion, liquid crystalline phase or coarse emulsion formulation (categorical outputs) from the water and oil proportion and HLB value of surfactants(s)/cosurfactant combination used (continuous inputs).

Data values from pseudo-ternary phase diagrams of blends of surfactants, or surfactant/co-surfactant, oil and water were used to develop a predictive NN model. Analysed samples representing the 20 different phase diagrams provided 5786 input–output data sets for the NNs. Each sample was labelled according to the proportions of surfactant blend used, calculated HLB value, oil, and water in the mixture, and matched with the nature of the phase structure found for that composition. i.e. microemulsion, coarse emulsion, or liquid crystalline, and a coexistence of two or three phases.

The results indicate that hybrid NNs have potential to predict the phase behaviour of colloidal systems with reasonable accuracy, with the model providing good quality results when dealing with categorical data. Although there were some errors in predicting the liquid crystalline phase, the microemulsion phase was predicted with high accuracy.

1. Introduction

Microemulsions are clear, low viscosity, thermodynamically stable dispersion of two immiscible liquids (oil and water) that are stabilized by surfactants. Due to their thermodynamic stability, microemulsions have been extensively investigated [1] as vehicles to deliver: (a) drugs with poor oral bioavailability [2]; (b) drugs that are susceptible to enzymatic degradation or (c) a combination of incompatible drugs with differing solubilities [3]. They form

Abbreviations: ANN, artificial neural network; BFGS, Broyden–Fletcher–Goldfarb–Shanno; CE, coarse emulsion; HNN, hybrid neural network; HLB, hydrophilic lipophilic balance; LC, liquid crystalline; LE, liquid crystalline phase and coarse emulsion; LFDS, low frequency dielectric spectroscopy; MC, coexistence of microemulsion and coarse emulsion; ME, microemulsion; ML, microemulsion and liquid crystalline; MLC, microemulsion, liquid crystalline and coarse emulsion; MLP, multilayer perceptron; O/W, oil-in-water emulsion; RBF, radial basis function; RBFT, radial basis function transform; W/O, water-in-oil emulsion.

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