Artificial neural network modeling on the polymer-electrolyte aqueous two-phase systems involving biomolecules

Yuqiu Chen[1], Xiaodong Liang[1], and Georgios Kontogeorgis[1]

[1]Technical University of Denmark

July 12, 2022

Abstract

In this work, modelling studies on the binodal curve behavior of polymer-electrolyte ATPS and the partitioning of biomolecules in these aqueous electrolyte solutions are carried out. First, a comprehensive database targeting the studied systems is established. Then, a novel modeling strategy that combines a well-known machine learning algorithm, i.e., artificial neural network (ANN) and group contribution (GC) method is proposed. Based on this modeling strategy, an ANN-GC model (ANN-GC model1) is built to describe the binodal curve behavior of polymer-electrolyte ATPS, while another ANN-GC model (ANN-GC model2) is developed to predict the partition of biomolecules in these biphasic systems. Furthermore, the obtained results also indicate that the tie-line length of polymer-electrolyte ATPS calculated from ANN-GC model1 can be directly used in ANN-GC model2 for predicting the partition performance coefficient of biomolecules in these ATPS.

Hosted file

`ANN modeling on ATPS-Biomolecuels_main content.docx` available at https://authorea.com/users/494793/articles/576757-artificial-neural-network-modeling-on-the-polymer-electrolyte-aqueous-two-phase-systems-involving-biomolecules