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A Newly Developed Tridimensional Neural Network for Prediction of the Phase Equilibria of Six Aqueous Two-Phase Systems

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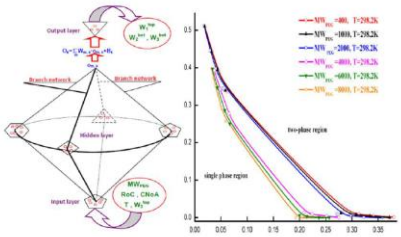
Graphical abstract



Highlights:

- A newly developed tridimensional neural network was proposed to represent the phase equilibria of six aqueous two-phase systems.
- The effects of the molecular weight of polymer, salt type and temperature on the phase behavior were incorporated in one model.
- The suggested model further improved the calculation accuracy.

Abstract: A newly developed tridimensional neural network (TRDNN) has been utilized to represent the phase equilibria of six polyethylene glycol (PEG)-inorganic salt aqueous two-phase systems (ATPSs). 18 data sets totaling 108 experimental data in the temperature range (298.2-318.2 K) were categorized into training, test and validation sets in order to teach the model about the input-output relationships and validate its predictive ability. The optimal configuration of the model was found to be {5, [3,4,5], 3} and the system error for the training process was determined as 0.0055. Results indicate that the TRDNN model has better prediction performance as compared to the two-dimensional model. The standard deviations corresponding to three data sets for the TRDNN model were 0.0057, 0.0068 and 0.0055, while those for the two-dimensional model were 0.0065, 0.0078 and 0.0062,