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Optimization of an Artificial Neural Network for Pure Component Parameters based on a Group Contribution Method of PC-SAFT EoS

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Abstract (less than 300 words)

In recent years, the perturbation theory-type equation of state (EoS), such as perturbed chain statical associating fluid theory (PC-SAFT) EoS [1], has been attracting attention owing to its applicability for wide molecular families including polymers and ionic liquids. The pure component parameters of the PC-SAFT EoS are generally obtained from liquid density and saturated vapor pressure. Unfortunately, these properties do not often exist. Therefore, a group contribution method (GCM) is used as one of the methods to obtain the pure component parameters. GCMs for parameters of the perturbation theory-type EoS have been reported [2, 3], whose high reliability was confirmed by numerous studies. However, the number of atomic groups covered is limited. Furthermore, it is impossible to predict when it comes to complex molecular structures. We introduced an artificial neural network (ANN), which can represent objects that are difficult to formulate, rather than the model of the GCM, because the model in the existing GCM is no longer able to manage enormous diversification of substances. Hence, a model to estimate the pure component parameters m, σ, and ε of the PC-SAFT EoS was developed. Furthermore, we tried to improve the estimation accuracy by optimizing the network structure and changing the input data. The results confirm that the model can determine the pure component parameters of PC-SAFT, which can estimate the liquid density, saturated vapor pressure, and critical properties. Furthermore, in each pure component parameters of the PC-SAFT EoS estimated using ANN, the estimation accuracy of the number of segments was lower than that of the other two parameters. We discussed this from several points of view and tried to improve the estimation accuracy of the number of segments.

References

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