# Influence of thermodynamically inconsistent data on modeling the solubilities of refrigerants in ionic liquids using an artificial neural network


- Fierro E.N.[a],
- Faundez C.A.[a],
- Munoz A.S.[b]



**Abstract**

In this work, a general thermodynamic consistency test is applied to analyze phase equilibrium data (PTx) for binary refrigerant and ionic liquid mixtures. The Valderrama-Patel-Teja (VPT) equation of state and the Kwak and Mansoori (KM) mixing rules are employed to correlate the solubility data of several refrigerants in different ionic liquids, and the Gibbs-Duhem equation is employed to check the thermodynamic consistency of six hundred forty-two experimental data points. The main purpose of this work is to analyze the influence of experimental data that are declared thermodynamically inconsistent on modeling the solubilities of refrigerants in ionic liquids using an artificial neural network. The results obtained via the test are classified into three categories: thermodynamically consistent, not fully consistent and thermodynamically inconsistent. Subsequently, a multilayer perceptron is trained to predict solubility in three cases: i) learning with isotherms that are declared thermodynamically consistent; ii) learning with isotherms, including those that are declared thermodynamically consistent and those that are not fully consistent; and iii) learning with all isotherms, even those that are declared thermodynamically inconsistent. For each case, the architecture, input combination and number of parameters necessary to achieve reasonable predictions are determined. The results show that the use of thermodynamically consistent and not fully consistent data is sufficient for finding an artificial neural network with a reasonable number of parameters.




**Author keywords**

Artificial neural network; Equation of state; Ionic liquids; Multilayer perceptron; Solubility; Thermodynamic consistency