Thermodynamic Properties Estimation for Pure and Binary Systems

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Reliable methods for estimating the vapor pressures of organic compounds are of increasing importance as a tool in predicting the behavior and fate of chemicals that are introduced into the environment. When a chemical like a CFC or HFC has been spilled, for example, we must know its approximate vapor pressure, in order to estimate its rate of evaporation. Without this information of vapor pressure, we can not get the Ozone Depletion Potential (ODP) and the Global Warming Potential (GWP) of these compounds.

The persistence of environmental hormones, insecticides, herbicides, and similar substances that have been absorbed in the soil is also highly dependent on Vapor Pressure. In the chemical engineering field, Vapor Pressure is one of the most important thermodynamic properties when designing a distillation tower in petroleum industry. In this case, not only vapor pressure but binary system’s activity coefficients are also needed.

There are several vapor pressure estimating schemes. The Lee-Kesler method needs Boiling Point (Tb), Critical Temperature (Tc) and Critical Pressure (Pc) to estimate vapor pressure. Riedel’s method, Riedel-Plank-Miller method and Asizawa method are also popular and need the same 3 properties.

When a property does not vary linearly with a set of parameters, the use of neural networks (NNs) in Quantitative structure property relationship (QSPR) studies has definite advantages over traditional methods. We have developed NNs based properties estimations schemes. We will show comparisons between Traditional Estimating methods and the NNs based method. For binary systems, an inter-molecular interaction parameter (Kij) estimation scheme can be used in Pen-Robinson type PVT relationships. Using this parameter, we can easily estimate azeotropes. Group Solution Model Theory “ASOG” results, which can calculate activity coefficients from their chemical structure will also be presented.
Prediction of Vapor Pressure

\[ \log(VP) = -0.4324*(Tr)^{1.69}*w^{0.18}*Sc^{0.68}*Tc^{0.08}\log(Pc)^{0.51} + 3.39*Tr^{0.17}*w^{0.04}*Sc^{0.19}*Tc^{0.04}\log(Pc)^{0.38} \]

\( VP \) = Vapor Pressure  
\( Tr \) = Measuring temperature / Critical temperature (Tc)  
\( Tb \) = Boiling Point, \( K = Tb/Tc \)  
\( Sc \) = \( K / (1-K) \)  
\( Pc \) = Critical Pressure