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Vapor Pressure Prediction Method for Pure Substances

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Abstract (less than 300 words)

In a newly proposed prediction method of vapor pressure, the parameters of the vapor pressure equation are directly determined using the parameter of the reference substance with one set of vapor pressure data, for example, boiling point data. A series of observed vapor pressure data of a substance shows linear relation between logarithm of measured vapor pressure and reciprocal value of its absolute temperature. In addition, the slope of the linear relation is almost same for homologous series. By using this slope of homologous substance, for the homologous substance of which vapor pressure is not observed, the intercept of the vapor pressure equation can be determined from the one set of vapor pressure data. As the vapor pressure equation, the Clapeyron and the Antoine equation are chosen. The method was applied for the following homologous substances; alcohols, acids, esters, ketones, organophosphors, pinenes, and silanes. The average absolute deviations (AAD) of these homologous substances were 0.615 and 0.709 kPa for the Antoine and the Clapeyron equations, respectively. The feature of the method is that it does not use any correlation, except that it uses a homologous substance as a reference substance. Therefore, unlike the other method, there is no error due to data correlation. The accuracy of the method depends on the difference in latent heat of vaporization between the substance to be estimated and the reference substance, that is, the difference in the slope of the vapor pressure expression equation. However, it depends on the selection of reference substance and temperature range to be used for prediction. Since this method is based on thermodynamically derived Clausius-Clapeyron relation, it is a widely and generally applicable method and there is no limitation by substance, temperature and pressure.