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New Low Vapor Pressure Estimation Method for Polar Compounds

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Vapor pressure estimation for polar compounds is very important in environmental chemistry. Most vapor pressure estimation equations are based on the Clausius-Clapeyron equation. Such equations are extremely accurate above the boiling point, but cannot be used for polar compounds around 1 Pa-100 Pa. A new polynomial expansion type of vapor pressure was developed. Such a non-linear expression has many solutions and the global minimal answer is difficult to obtain. The Genetic Algorithm (GA) was applied to determine the coefficients of the polynomial expansion equation. The accuracy of this polynomial expansion equation for vapor pressure is much better than the Riedel equation under the boiling point for polar compounds. This method was also applied for acentric factor estimation and an estimation equation with better accuracy than the Edmister equation is proposed.

Keywords: [Vapor pressure estimation](#), [Polynomial equation](#), [Genetic algorithm](#), [Acentric factor](#), [Riedel equation](#)



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