Fitting Vapor Pressure - Temperature Data: Simplicity and Unintended Consequences

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ABSTRACT

The (1, 1.5, 3, 6) Wagner vapor pressure equation has gained acceptance in a variety of applications, e.g. in various software packages designed to 'simulate' chemical engineering processes. While this equation can fit vapor pressure data over the entire temperature range including the vicinity of the critical point, indiscriminate use of this equation can lead to substantial extrapolation errors and erroneous enthalpies of vaporization. Several examples of vapor pressure fits compare results obtained from the (1, 1.5, 3, 6) Wagner equation with other equations constrained to fit the lower and higher pressure limits.