

Property Estimation from Family Plots: A Case Study of the *n*-Alkane Family

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Accurate experimental data can be effectively used as a basis for predicting property values for other members of well-defined families, especially if reliable data exist for several compounds belonging to the same family. Accurate predictions of “constant” properties such as critical properties, acentric factor, normal boiling point temperature, etc. can be obtained by extrapolation or interpolation of “family curves”. Similarly, experimental values of temperature-dependant properties such as vapor pressure, heat of vaporization, liquid density, etc. can be evaluated in order to accurately predict the shape and magnitude of these properties for other members of the same family. As many thermodynamic and physical properties are inter-related, it is essential that properties predicted from “family plots” are internally consistent. In this paper we present a case study with the *n*-alkane family. As the interest in larger alkanes continues to increase, the ability to accurately predict property values for such compounds becomes increasingly important. Accurate extrapolation well beyond the range of reliable experimental data becomes difficult and the internal consistency of the resulting properties relies upon sound theory and judgment. This case study demonstrates the process that we used to obtain a consistent, reliable set of properties for *n*-alkanes up to *n*-octacontane. A similar process can be used to expand the range of other well-defined families.