Use of Transformed Correlations to Help Screen & Populate Properties within Databanks

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Thermophysical property databanks are often sparsely populated with properties. Too frequently, temperature-dependent property fits within databanks contain entry errors or other errors which may have eluded earlier detection. While many organizations, such as DIPPR, employ quality checks to help eliminate these kinds of defects within their databanks, what we propose here is a more systematic use of transformed correlations that automatically "fit" properties to desired equation forms used within a database. This approach is most applicable to properties that can be estimated by relatively simple Group Contribution (GC) or Corresponding States Principle (CSP) methods. Dow Corning is currently applying this approach to help convert non-standard equation forms within its internal database to more universally accepted equations. As an example, the 1988 Harrison & Seaton (H&S) correlation for ideal gas heat capacity (ICP) has been converted into a transformation. The method was originally published as a tabular atomic GC method where the groups are a function of temperature. The fit of this table faithfully reproduces the H&S table and allows one to automatically convert lists of empirical formulas into coefficients for the Aly & Lee equation. When we compared the transformation fits for components in our database with the original database fits, numerous discrepancies were identified including typos and unit conversions; however, we also discovered problems with some published ICP spectroscopic data in the literature. The transform also pointed out a scaling problem with ICP data for dimethylsiloxanes in the DIPPR database that were estimated by *ab initio* methods.