Pareto-Optimum Parameter Estimation in Thermodynamic Correlations

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A reliable estimate of model parameters in thermodynamic correlations and simulations is an important requirement in many applications. A transition from a real phenomenon to its model entails the appearance of uncertainty caused by the statistical pattern of experimental information, inadequacy and ambiguity of implemented models, etc. Due to the estimation of parameters from experimental data, which are generated by different experimental units, the measured data have, as a rule, different dimensions, physical meanings, and statistical distributions. A conflicting situation results when the set of parameters determined according to one category of data does not correspond to parameters from other data sources. Therefore, the conflict appears in the model parameter estimation, and it is desirable to reduce arising uncertainty by the simultaneous consideration of all data fitness criteria for each property.

The aim of the present work is to include uncertainty in conventional methods of parameter estimation in order to find solutions that simultaneously meet various data fitting criteria.

Complementary models (anti-optimization, game theoretical, and fuzzy set) of uncertainty are analyzed as a source of conflict between thermodynamically inconsistent data. The problem of optimum parameter estimation in thermodynamic models considering the uncertainty is formulated as a multicriteria problem of mathematical programming. The first step in the solution of a multicriteria problem is an exploration of the Pareto set, i.e., the domain in the permissible parameter space where the value of any criterion cannot be improved without the value of other criteria being worsened. The diverse computational methods of the Pareto-optimum parameter estimation and different (crisp and fuzzy) convolution schemes to reduce a vector criterion into a scalar one are given. The novel approach to Pareto-optimum estimation of the equation of state parameters, using different conflicting data sets (simultaneous description of the phase equilibria and critical line data in binary mixtures, thermodynamically consistent description of inhomogeneous data, and other inconsistency problems arising in the modeling of thermophysical properties of substances) is considered.