Automatic Fitting of Refrigerant Thermodynamic Models

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In recent years significant progress has been made towards automatic fitting of mixture parameters and departure functions using global stochastic optimization. Highly accurate models have been developed based on homogeneous density, phase equilibria, and speed of sound data, especially in the case of well-measured refrigerant-containing binary pairs. The process is mostly automated.

This process has matured to the point that a Python package entitled temo has been released which includes the necessary functionality to fit such models as part of a processing pipeline. First, experimental data are extracted from the NIST SOURCE database with an in-house interface. The data files are converted to harmonized file formats along with bibliographic information. Then, a user-defined set of interaction parameters and/or departure functions are fit with temo.

The fitting process is reproducible, as the driving script is a few hundred lines of code and uses publicly available functionality from the temo and teqp libraries. The development of highly reliable algorithms for tracing isotherms and isobars for binary mixtures is at the very heart of this technique.

The main themes of this work are twofold: 1) to evaluate the estimation schemes and provide guidance on which estimation schemes are most suitable for a given mixture and 2) to fit binary interaction parameters and departure functions depending on the availability of high-quality data. There are not too many systems remaining where the experimental data warrants the development of a departure function.

Ultimately, where warranted, these models will replace the existing models in NIST REFPROP.