A Reference Database for Benchmarking Equations of State

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While people are continuously developing equations of state sharing more or less the same objectives, that are, be able to reproduce phase-equilibrium and energetic property data of a large (if not, the largest) possible set of pure compounds and related mixtures, there is currently no means to evaluate all these models on the same and fair basis. Any thermodynamic model developer might expect the existence of a reference database for benchmarking his model, including consistent experimental data for a wide number of properties and systems deemed as well representative of the variety of molecular interactions occurring in nature. Indeed, as stated by Hendriks et al (Ind. Eng. Chem. Res. 2010, 49, 11131–11141) “there are databases (NIST-TRC, Dechema-Detherm) that are used by individuals [but] their use is still not widespread enough.” Therefore, new published models are not evaluated on the same experimental datasets, making any kind of comparison almost impossible. Our work is intended to fill this gap by proposing both a reference database of binary systems data and a procedure for evaluating deviations between model correlations and data. For selecting the data present in our database, we developed first a methodology to predict associative behaviors in solution for both pure compounds and binary systems from their chemical structure (associating phenomena being considered as an important indicator of molecular interactions in binary systems). This led us to define 9 families of binary systems ranging from non-associating to highly-associating systems and containing both ideal and non-ideal systems (well illustrative of enthalpic and entropic effects). For each system, accurate, reliable, and thermodynamically-consistent data associated with various kinds of thermodynamic properties (vapor-liquid, liquid-liquid, vapor-liquid-liquid equilibrium data, critical points, azeotropic points, enthalpy, and heat-capacity of mixing data …) were included. In the end, we used our database, made up of nearly 220 binary systems, to benchmark the Peng-Robinson equation of state.