Empirical Fundamental Equations of State Correlations Based on Hybrid Datasets

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The process engineering industry is in an ever increasing demand for thermodynamic data that cannot be satisfied exclusively with experimental measurements due to cost and time inefficiency. Moreover, often extreme thermodynamic conditions or hazardous fluids have to be considered. The primary purpose of empirical fundamental equation of state correlations (FEOS) is to extend the range of available experimental data by offering interpolation and extrapolation capability. A FEOS can be expressed in forms of various thermodynamic potentials. A thermodynamic potential has ability that every other thermodynamic property can be obtained as a combination of its derivatives with respect to its natural variables. The construction of a FEOS requires less data than the amount that would be needed to map the entire fluid region of technological relevance. Nonetheless, FEOS exist only for a very limited subset of the pure compounds that are in technological use. For mixtures, where the range of required data increases drastically with the number of components, the situation is much worse. Molecular simulation has evolved to a point where it can contribute effectively to thermodynamic data retrieval. Its predictive capability is limited only by the molecular interaction model that represents the investigated substance, molecular simulation can straightforwardly target any state point of interest while the associated financial cost and time requirement is only a fraction than that of a corresponding laboratory measurement. Besides the usual thermodynamic properties obtained from measurements, molecular simulation can directly deliver the derivatives of the FEOS with respect to its natural variables, making fitting procedures simpler.