Industrial Requirements for Thermodynamics and Transport Properties

This work reports the results of an investigation on industrial requirements for thermodynamic and transport properties carried out by the Working Party on Thermodynamic and Transport properties (http://www.wp-ttp.dk/) of the European Federation of Chemical Engineering, EFCE (http://www.efce.info/). A carefully designed questionnaire was sent to a number of key technical people in companies in the oil and gas, chemicals, and pharmaceutical/biotechnology sectors. Twenty-eight companies have provided answers which formed the basis for the analysis presented here. A number of previous reviews, specifically addressed to or written by industrial colleagues, are discussed initially. This provides the context of the survey and material with which the results of the survey can be compared. The results of the survey have been divided into the themes: data, models, systems, properties, education, and collaboration. The main results are as follows. There is (still) an acute need for accurate, reliable, and thermodynamically consistent experimental data. Quality is more important than quantity. Similarly, there is a great need for reliable predictive, rather than correlative, models covering a wide range of compositions, temperatures, and pressures and capable of predicting primary (phase equilibrium) and secondary (enthalpy, heat capacity, etc.) properties. It is clear that the ideal of a single model covering all requirements is not achievable, but there is a consensus that this ideal should still provide the direction for future development. The use of new methods, such as SAFT, is increasing, but they are not yet in position to replace traditional methods such as cubic equations of state (especially in oil and gas industry) and the UNIFAC group contribution approach. A common problem with novel methods is lack of standardization, reference data, and correct and transparent implementations, especially in commercially available simulation programs. The survey indicates a great variety of systems where further work is required. For instance, for electrolyte systems better models are needed, capable of describing all types of phase behavior and mixtures with other types of components. There is also a lack of data and methods for larger complex molecules. Compared with the previous reviews, complex mixtures containing carbon dioxide associated with a wide range of applications, such as capture, transport, and storage are becoming interesting to a number of survey participants. Despite the academic success of molecular simulation techniques, the survey does not indicate great interest in it or its future development. Algorithms appear to be a neglected area, but improvements are still needed especially for multiphase reactive systems (simultaneous chemical and physical equilibrium). Education in thermodynamics is perceived as key, for the future application of thermodynamics in the industry. A number of suggestions for improvement were made at all three levels (undergraduate, postgraduate, and professional development) indicating that the education is correctly perceived as an ongoing process.