An Integrated Methodology for Advanced Thermodynamics in Process Modelling

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The accurate prediction of the thermophysical properties of substances is of prime importance for the design of high-performance materials and the design and operation of efficient chemical processes. As the chemical industry increasingly focuses on high value-added complex materials and faces tightening environmental regulations, thermodynamic models that can reliably represent highly non-ideal systems over wide ranges of operating conditions are becoming an invaluable asset (see, for instance, [i]). The well-known cubic equations of state (Redlich-Kwong, Peng-Robinson, and their variations), which have been the staple of process simulators since their inception, are appropriate for small, roughly spherical molecules. However, they cannot offer the necessary accuracy for the complex systems that are at the core of many of the process industry's current activities. The process engineering community must now capitalise on the fundamental progress of thermodynamic models over the last few years.

Recent attempts at developing equations of state have been based on a more rigorous statistical mechanical framework. Because of their sound theoretical basis, such techniques are more predictive than the empirical approaches, and they can be used to extrapolate from a relatively small amount of information. They have been particularly successful at modelling highly polar, nonspherical-amphiphilic and charged molecules such as hydrogen fluoride, surfactants, and electrolytes.

The SAFT equation of state [ii] represents a good example of such an approach. The accurate predictions provided for associating systems by the SAFT framework have been used for process design calculations by a number of companies. For instance, the SAFT models developed by Professor Jackson's group have provided thermophysical data for the production of replacement refrigerants at ICI Runcorn [iii]. At the large end of the molecular scale, SAFT models have attracted great interest from Unilever, ICI and BP Amoco in the modelling of aqueous micellar solutions of alkyl polyoxyethylene (CiEj) surfactants [iv], used as soaps, detergents and lubricants and in oil extraction, where they have helped extend the lifetime of oil wells by up to a factor of five. The predictive accuracy, versatility and firm molecular foundation of the state-of-the-art SAFT approach have made it a likely candidate to replace more traditional thermodynamic models in process design.

References

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